

STIC-EIC1600/2900

262753

LB

From: Zarek, Paul
Sent: Friday, June 06, 2008 12:25 PM
To: STIC-EIC1600/2900
Subject: Structure search for 10/598508

Hello,

Would you please do a structure search of the attached structure. It's for application 10/598,508. I am attempting to break unity of a national stage phase of a 371 application. The filing date is 03/03/2004.

Please let me know if you have any questions/concerns. Thanks,

Paul E. Zarek
Patent Examiner
CIAC 3003
Art Unit 4161
571.270.5754
paul.zarek@uspto.gov

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6/6/2008

=> file registry

FILE 'REGISTRY' ENTERED AT 13:45:21 ON 10 JUN 2008

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Property values tagged with IC are from the ZIC/VINITI data file

10/598508

provided by InfoChem.

STRUCTURE FILE UPDATES: 9 JUN 2008 HIGHEST RN 1026855-74-2
DICTIONARY FILE UPDATES: 9 JUN 2008 HIGHEST RN 1026855-74-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

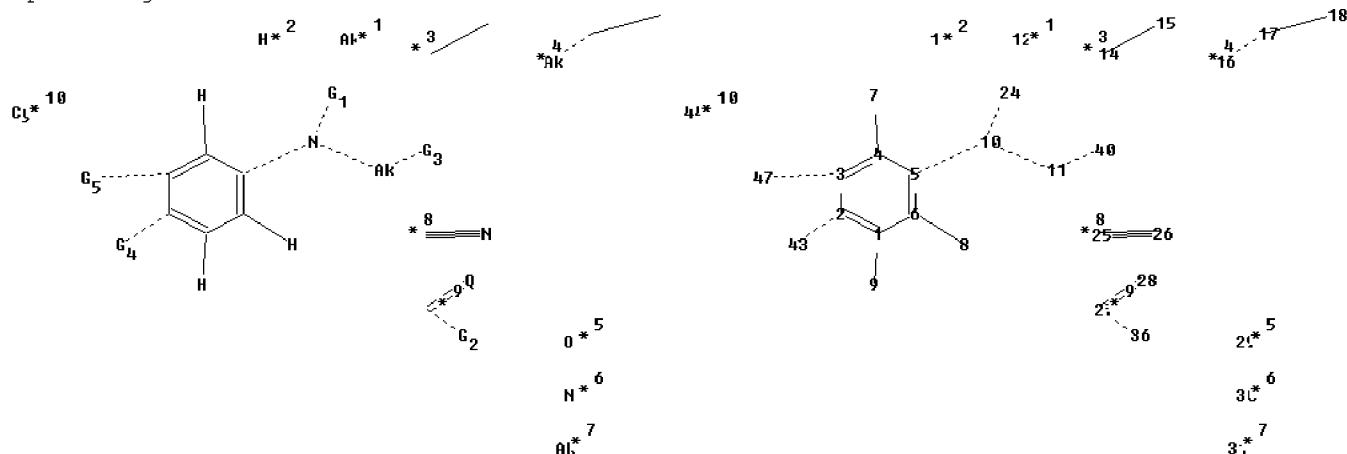
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
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on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

Uploading L1b.str



chain nodes :

7 8 9 10 11 12 13 16 24 25 26 27 28 29 31 36 40 43 44 47

ring nodes :

1 2 3 4 5 6 14 15 17 18

ring/chain nodes :

30

chain bonds :

1-9 2-43 3-47 4-7 5-10 6-8 10-11 10-24 11-40 16-17 25-26 27-28 27-36

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 17-18

exact/norm bonds :

2-43 3-47 5-10 10-11 10-24 11-40 16-17 25-26 27-28 27-36

exact bonds :

1-9 4-7 6-8 14-15 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4]

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G2:[*5],[*6],[*7]

G3:[*8],[*9]

G4:CN,NO2,X

G5:CN,NO2,O,X,Ak,[*10]

Connectivity :

11:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom

24:CLASS 25:CLASS

26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 36:CLASS 40:CLASS

43:CLASS 44:Atom

47:CLASS

Generic attributes :

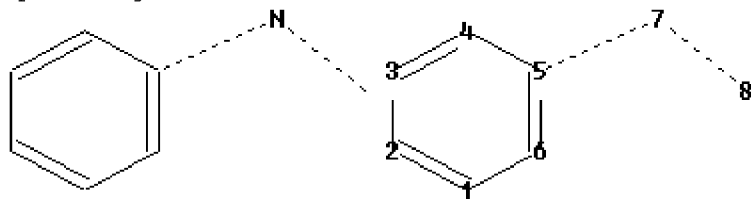
11:

Saturation : Saturated

44:

Saturation : Unsaturated

Uploading L3b.str



chain nodes :

7 8

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

5-7 7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Connectivity :

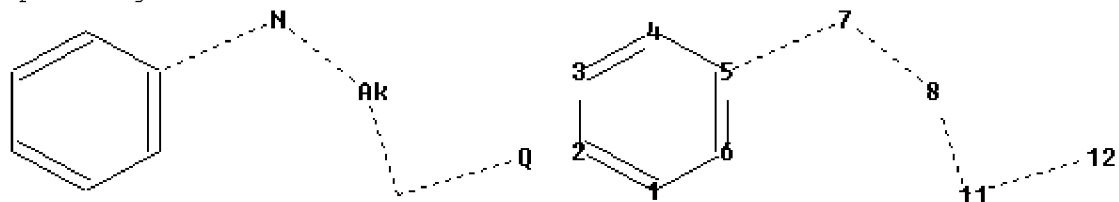
1:2 E exact RC ring/chain 4:2 E exact RC ring/chain 6:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS

10/598508

Uploading L4b.str



chain nodes :

7 8 11 12

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 7-8 8-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

5-7 7-8 8-11 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Connectivity :

1:2 E exact RC ring/chain 4:2 E exact RC ring/chain 6:2 E exact RC ring/chain

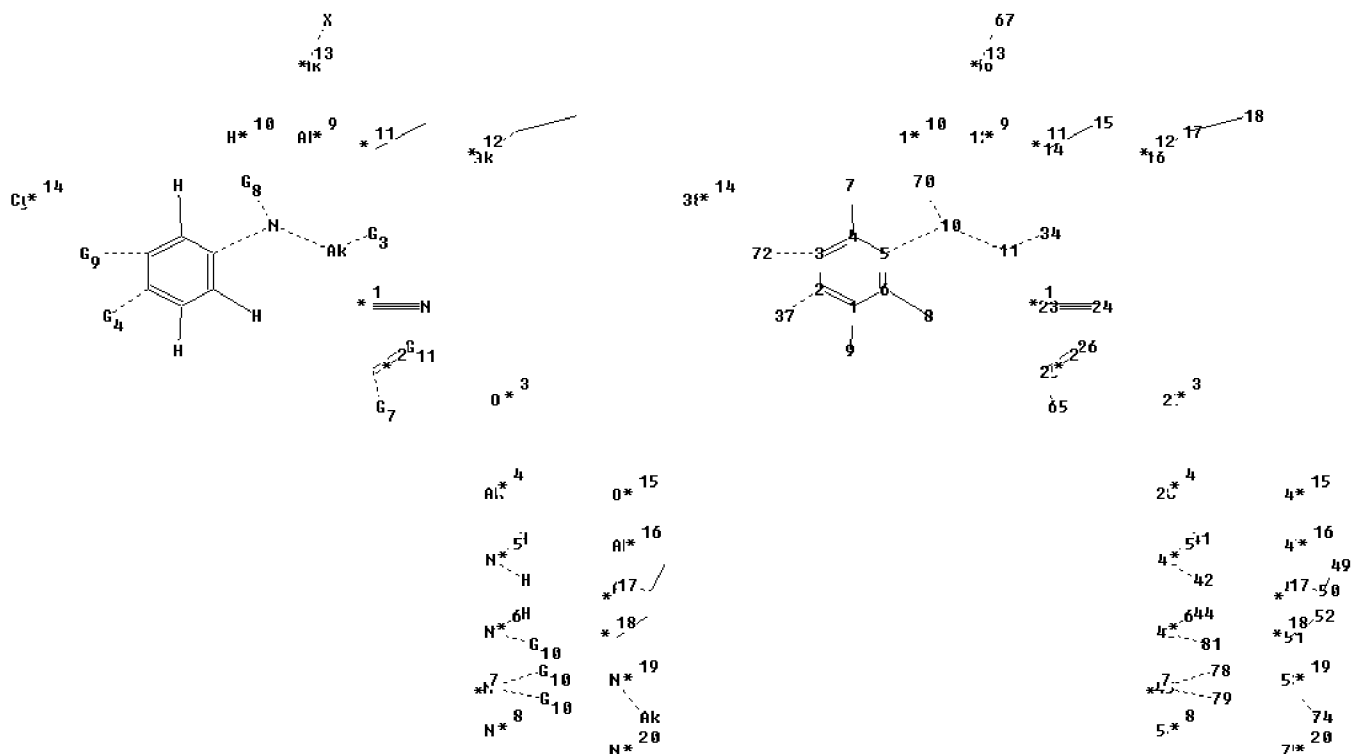
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 11:CLASS

12:CLASS

Uploading L21b.str

10/598508



chain nodes :

7 8 9 10 11 12 13 16 23 24 25 26 27 28 34 37 38 40 41 42 43
44 45 46 47 48 53 65 66 67 70 72 74 75 78 79 81

ring nodes :

1 2 3 4 5 6 14 15 17 18 49 50 51 52 54

chain bonds :

1-9 2-37 3-72 4-7 5-10 6-8 10-11 10-70 11-34 16-17 23-24 25-26 25-65
40-41 40-42 43-44 43-81 45-78 45-79 48-50 53-74 66-67

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 17-18 49-50 51-52

exact/norm bonds :

2-37 3-72 5-10 10-11 10-70 11-34 16-17 23-24 25-26 25-65 40-41 40-42
43-44 43-81 45-78 45-79 48-50 53-74 66-67

exact bonds :

1-9 4-7 6-8 14-15 17-18 49-50 51-52

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G3:[*1],[*2]

G4:CN,NO2,X

G7:[*3],[*4],[*5],[*6],[*7],[*8]

G8:[*9],[*10],[*11],[*12],[*13]

G9:CN,NO2,X,O,[*9],[*14],[*13]

G10:[*15],[*16],[*17],[*18],[*19],[*20]

10/598508

G11:O,S,[*19],[*20]

Connectivity :

12:1 E exact RC ring/chain 47:1 E exact RC ring/chain 74:1 E exact RC ring/chain

75:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom

23:CLASS 24:CLASS

25:CLASS 26:CLASS 27:CLASS 28:CLASS 34:CLASS 37:CLASS 38:Atom 40:CLASS

41:CLASS 42:CLASS

43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:Atom 50:Atom

51:Atom 52:Atom 53:CLASS

54:Atom 65:CLASS 66:CLASS 67:CLASS 70:CLASS 72:CLASS 74:CLASS 75:CLASS

78:CLASS 79:CLASS

81:CLASS

Generic attributes :

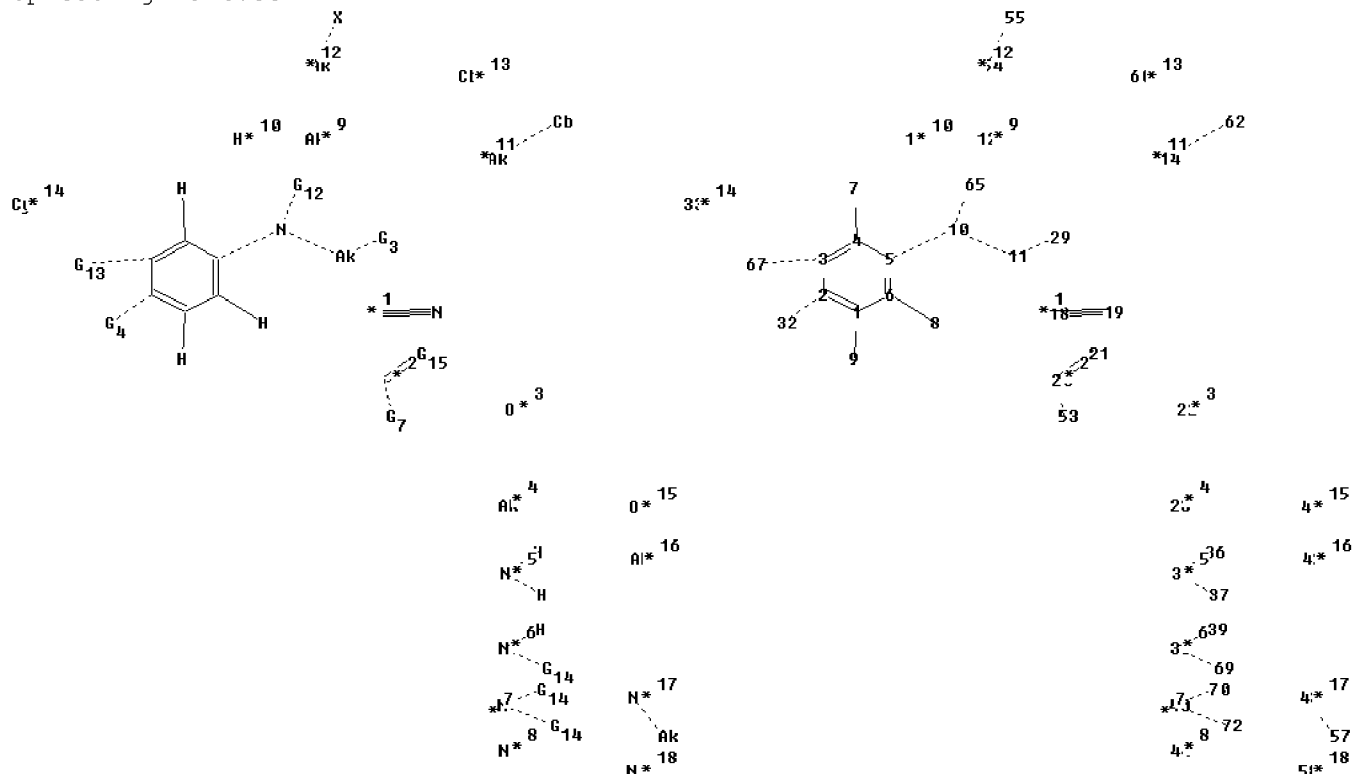
11:

Saturation : Saturated

38:

Saturation : Unsaturated

Uploading L52b.str



chain nodes :

7 8 9 10 11 12 13 14 18 19 20 21 22 23 29 32 33 35 36 37 38
39 40 41 42 43 53 54 55 57 58 60 62 65 67 69 70 72

ring nodes :

1 2 3 4 5 6 44

chain bonds :

10/598508

1-9 2-32 3-67 4-7 5-10 6-8 10-11 10-65 11-29 14-62 18-19 20-21 20-53
35-36 35-37 38-39 38-69 40-70 40-72 43-57 54-55

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

2-32 3-67 5-10 10-11 10-65 11-29 14-62 18-19 20-21 20-53 35-36 35-37
38-39 38-69 40-70 40-72 43-57 54-55

exact bonds :

1-9 4-7 6-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G3:[*1],[*2]

G4:CN,NO2,X

G7:[*3],[*4],[*5],[*6],[*7],[*8]

G12:[*9],[*10],[*11],[*12],[*13]

G13:O,CN,NO2,X,[*9],[*14],[*12]

G14:[*11],[*15],[*16],[*17],[*18],[*13]

G15:O,S,[*17],[*18]

Connectivity :

12:1 E exact RC ring/chain 14:2 E exact RC ring/chain 23:1 E exact RC ring/chain
33:1 E exact RC ring/chain 42:1 E exact RC ring/chain 57:1 E exact RC ring/chain
60:1 E exact

RC ring/chain 62:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS

22:CLASS 23:CLASS

29:CLASS 32:CLASS 33:Atom 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS

40:CLASS 41:CLASS

42:CLASS 43:CLASS 44:Atom 53:CLASS 54:CLASS 55:CLASS 57:CLASS 58:CLASS

60:CLASS 62:Atom

65:CLASS 67:CLASS 69:CLASS 70:CLASS 72:CLASS

Generic attributes :

11:

Saturation : Saturated

33:

Saturation : Unsaturated

=> file zcaplus

FILE 'ZCAPLUS' ENTERED AT 13:45:28 ON 10 JUN 2008

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FILE COVERS 1907 - 10 Jun 2008 VOL 148 ISS 24
FILE LAST UPDATED: 9 Jun 2008 (20080609/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

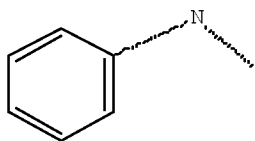
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L58
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

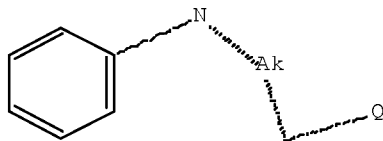
Structure attributes must be viewed using STN Express query preparation.

L2 SCR 1867
L3 STR



Structure attributes must be viewed using STN Express query preparation.

L4 STR



Structure attributes must be viewed using STN Express query preparation.

L5 SCR 616
L6 SCR 1944
L7 SCR 1992
L8 SCR 2004 OR 2021 OR 1993
L9 SCR 868
L10 SCR 877

10/598508

L11 2640 SEA FILE=REGISTRY SSS FUL (L1 AND L3 AND L4) AND (L2 AND L5
AND L6 AND L7 AND L8 AND L9 AND L10)
L21 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L23 654 SEA FILE=REGISTRY SUB=L11 SSS FUL L21
L26 1 SEA FILE=REGISTRY ABB=ON PLU=ON 14108-81-7
L27 1 SEA FILE=REGISTRY ABB=ON PLU=ON 65051-17-4
L28 1 SEA FILE=REGISTRY ABB=ON PLU=ON 22212-58-4
L29 1 SEA FILE=REGISTRY ABB=ON PLU=ON 22212-57-3
L30 1 SEA FILE=REGISTRY ABB=ON PLU=ON 33878-52-3
L31 1 SEA FILE=REGISTRY ABB=ON PLU=ON 33878-51-2
L32 1 SEA FILE=REGISTRY ABB=ON PLU=ON 28363-22-6
L33 1 SEA FILE=REGISTRY ABB=ON PLU=ON 52756-23-7
L34 1 SEA FILE=REGISTRY ABB=ON PLU=ON 52756-26-0
L52 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L54 613 SEA FILE=REGISTRY SUB=L23 SSS FUL L52
L57 604 SEA FILE=REGISTRY ABB=ON PLU=ON L54NOT (L26 OR L27 OR L28
OR L29 OR L30 OR L31 OR L32 OR L33 OR L34)
L58 131 SEA FILE=ZCAPLUS ABB=ON PLU=ON L57

=> d ibib abs hitstr L58 tot; d ibib abs hitstr L64 21; d ibib abs hitstr L65 16; d
ibib abs hitstr L66 15; d ibib abs hitstr L67 14; d ibib abs hitstr L68 10; d ibib
abs hitstr L69 9; d ibib abs hitstr L70 8; d ibib abs hitstr L71 7; d ibib abs
hitstr L72 7

L58 ANSWER 1 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:99761 ZCAPLUS Full-text

DOCUMENT NUMBER: 148:191943

TITLE: Preparation of N-[1-biphenyl-yl-(morpholinyl- and
pyrrolidinyl)ethyl]glycinamide derivatives as
antagonists of urotensin II

INVENTOR(S): Neeb, Michael J.; Sehon, Clark A.; Viet, Andrew Q.;
Goodman, Krista B.; Wang, Gren Z.

PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 287pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2008011551	A1	20080124	WO 2007-US73951	20070720
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,			

10/598508

IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM

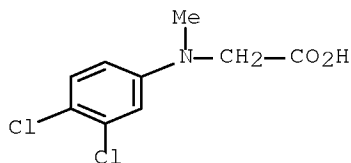
US 20080021023 A1 20080124 US 2007-780584 20070720
PRIORITY APPLN. INFO.: US 2006-832176P P 20060720
US 2006-870202P P 20061215
OTHER SOURCE(S): MARPAT 148:191943
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; R1 = (un)substituted Ph, Q; A = (CH₂)_n; n = 1-2; R2 = H, halo, O-C1-3 alkyl, NHC(O)-C1-3 alkyl, NHSO₂-C1-3 alkyl, NHSO₂Ph, NHC(O)-C3-6 cycloalkyl, NHC(O)Ph; R3 = C1-3 alkyl, C3-6 cycloalkyl; R4, R5, R6 = independently H or Me; X = O, a bond; B = Q1, Q2, Q3, Q4, Q5, Q6; R12 = H, C1-3 alkyl, CH₂CN, (CH₂)mOMe, CH₂C(O)NH₂, (CH₂)mOH; R13 = H, halo, C1-3 alkyl, CF₃, O-C1-3 alkyl; m = 2 or 3; R14 = H, halo, C1-3 alkyl, O-C1-3 alkyl, OCF₃, CF₃, C(O)NR₁₅R₁₆, or C(O)O-C1-3 alkyl; R15, R16 = independently H, C1-3 alkyl, C3-6 cycloalkyl, or Ph] or pharmaceutically acceptable salts thereof are prepared These compds. are antagonists of urotensin II (no data) and useful for treating congestive heart failure, stroke, ischemic heart disease, angina, myocardial ischemia, overactive bladder, or cardiac arrhythmia. Thus, [1-(4-biphenyl)-2-(4-morpholinyl)ethyl]methylamine was added to a solution of N-(6,7-dibromo-3-oxo-2,3-dihydro-4H-1,4-benzoxazin-4-yl)acetic acid, (benzotriazol-1-yl)oxytris(dimethylamino)phosphonium hexafluorophosphate (BOP), and Et₃N in CH₂Cl₂ and stirred at room temperature for 3 h to give N-[1-(1,1'-biphenyl-4-yl)-2-(4-morpholinyl)ethyl]-2-(6,7-dibromo-3-oxo-2,3-dihydro-4H-1,4-benzoxazin-4-yl)-N-methylacetamide (II).

IT 1003872-82-9P, N-(3,4-Dichlorophenyl)-N-methylglycine lithium salt
1003878-18-9P, Ethyl N-(3,4-dichlorophenyl)-N-methylglycinate
1003878-61-2P 1003878-62-3P, N-(3,4-Dichlorophenyl)-2-methylalanine lithium salt
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of N-[1-biphenyl-(morpholinyl- and pyrrolidinyl)ethyl]glycinamide derivs. as antagonists of urotensin II)

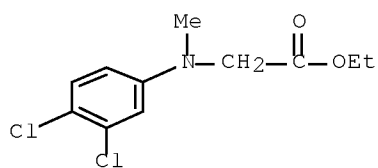
RN 1003872-82-9 ZCAPLUS
CN Glycine, N-(3,4-dichlorophenyl)-N-methyl-, lithium salt (1:1) (CA INDEX NAME)



● Li

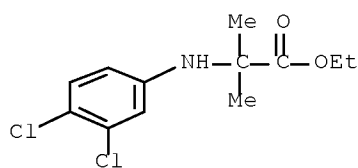
RN 1003878-18-9 ZCAPLUS
CN Glycine, N-(3,4-dichlorophenyl)-N-methyl-, ethyl ester (CA INDEX NAME)

10/598508



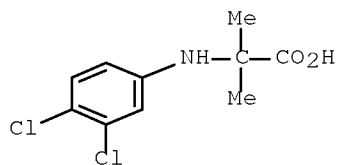
RN 1003878-61-2 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-2-methyl-, ethyl ester (CA INDEX NAME)



RN 1003878-62-3 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-2-methyl-, lithium salt (1:1) (CA INDEX NAME)



● Li

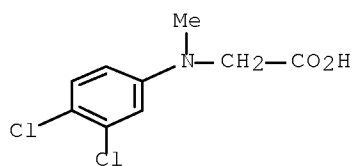
IT 1003878-30-5, N-(3,4-Dichlorophenyl)-N-methylglycine

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; preparation of N-[1-biphenyl-1-(morpholinyl- and pyrrolidinyl)ethyl]glycinamide derivs. as antagonists of urotensin II)

RN 1003878-30-5 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)-N-methyl- (CA INDEX NAME)

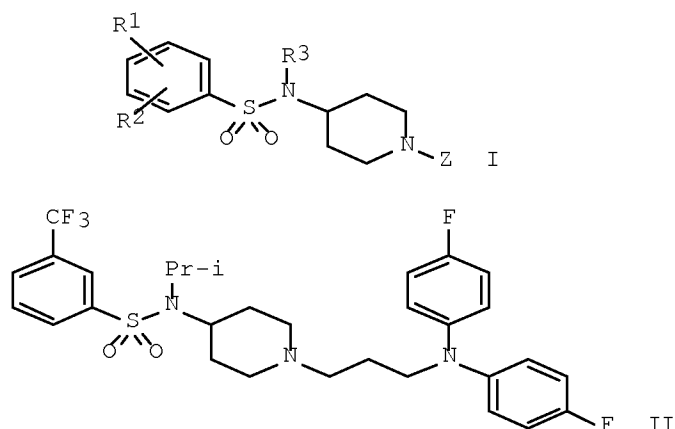


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 2 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:1204104 ZCAPLUS Full-text
 DOCUMENT NUMBER: 147:502239
 TITLE: Benzenesulfonamide compounds and their use as blockers
 of calcium channels and their preparation and use in
 the treatment of pain
 INVENTOR(S): Yao, Jiangchao; Shao, Bin; Kyle, Donald J.; Sha,
 Deyou; Chen, Zhengming; Islam, Khondaker; Zhou,
 Xiaoming
 PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg
 SOURCE: PCT Int. Appl., 332pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007118853	A1	20071025	WO 2007-EP53620	20070413
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: US 2006-791414P P 20060413
 OTHER SOURCE(S): MARPAT 147:502239
 GI



AB The invention relates to piperidinyll and hexahydroazepinyll compds. of formula I and pharmaceutically acceptable salts, prodrugs, or solvates thereof. The invention is also directed to the use compds. of formula I to treat, prevent or ameliorate a disorder responsive to the blockade of calcium channels, and particularly N-type calcium channels. Compds. of the invention are especially useful for treating pain. Compds. of formula I wherein R1 and R2 are independently H, (halo)alkyl, halo, (halo)alkoxy, CN, NO₂, amino, aminoalkyl, (di)alkylamino and OH; R3 is H, alkyl, alkenyl, cycloalkyl(alkyl), alkoxyalkyl, hydroxyalkyl, tetrahydrofuranyl, etc.; Z is (un)substituted acyl, (un)substituted alkyl, (un)substituted sulfonyl; and their pharmaceutically acceptable salts, prodrugs, and solvates thereof, are claimed. Example compound II was prepared by N-alkylation of N-isopropyl-N-(piperidin-4-yl) 3-trifluoromethylbenzenesulfonamide with 3-[bis(4-fluorophenyl)amino]propyl methanesulfonate. All the invention compds. were evaluated for their calcium channel modulatory activity. From the assay, it was determined that compound II exhibited IC₅₀ values of about 100 μM or less.

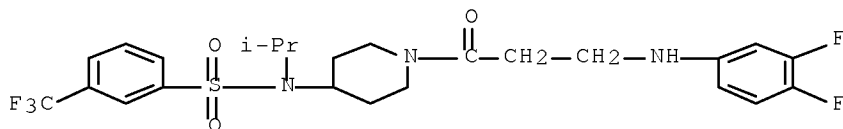
IT 955033-65-5P 955033-71-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzenesulfonamide compds. as calcium channel blockers useful in the treatment of pain)

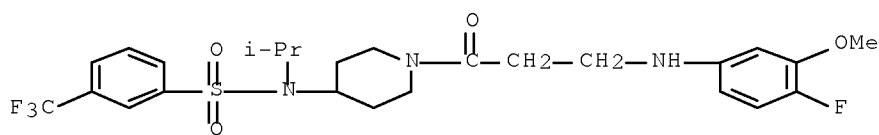
RN 955033-65-5 ZCAPLUS

CN Benzenesulfonamide, N-[1-[3-[(3,4-difluorophenyl)amino]-1-oxopropyl]-4-piperidinyll]-N-(1-methylethyl)-3-(trifluoromethyl)- (CA INDEX NAME)



RN 955033-71-3 ZCAPLUS

CN Benzenesulfonamide, N-[1-[3-[(4-fluoro-3-methoxyphenyl)amino]-1-oxopropyl]-4-piperidinyll]-N-(1-methylethyl)-3-(trifluoromethyl)- (CA INDEX NAME)

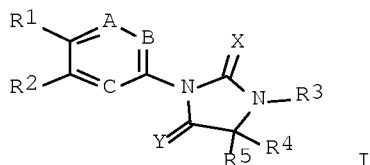


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 3 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:1040613 ZCAPLUS Full-text
 DOCUMENT NUMBER: 147:427336
 TITLE: Androgen receptor-regulator hydantoin derivatives and its application
 INVENTOR(S): Chen, Degui
 PATENT ASSIGNEE(S): Peop. Rep. China
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 34pp.
 CODEN: CNXXEV
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101032483	A	20070912	CN 2006-10067719	20060309
PRIORITY APPLN. INFO.:			CN 2006-10067719	20060309
OTHER SOURCE(S):			CASREACT 147:427336; MARPAT 147:427336	

GI



AB The invention relates to androgen receptor-regulator hydantoin derivs. I (R1 = CN, NO2, OH, SO-R3 or SO2-R3; R2 = halogen, halogen substitute, (un)saturated alkyl or its substitute; R3 = H, halogen, halogen substitute, (un)saturated alkyl, aryl, heterocyclic ring, arylalkyl; R4 and R5 = H, halogen, halogen substitute, (un)saturated alkyl or its substitute, oxyalkyl, nitroalkyl, or thioalkyl, which may be linked to form ring; A, B and C = C or N and at least one of them is N; X and Y = S, O or substituted amino). The hydantoin derivs. or their salts can be used for treating prostate cancer, which is hormone-sensitive or drug-resistant in hormone therapy, other androgen receptor-related diseases such as breast cancer, hyperplasia of prostate, hirsutism, comedo, calvities, muscle failure, hypogonadism, osteoporosis, high

10/598508

cholesteric, male sterility, etc., and central nerve-related disease such as low erotism, melancholia, etc.

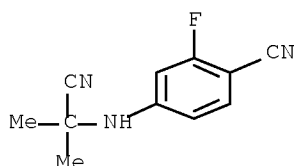
IT 951753-55-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of hydantoin derivs. and application as androgen receptor modulator)

RN 951753-55-2 ZCAPLUS

CN Benzonitrile, 4-[(1-cyano-1-methylethyl)amino]-2-fluoro- (CA INDEX NAME)



L58 ANSWER 4 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:730896 ZCAPLUS Full-text

DOCUMENT NUMBER: 147:143468

TITLE: Heterocyclic derivatives as modulators of ion channels and their preparation, pharmaceutical compositions and use in the treatment of diseases

INVENTOR(S): Wilson, Dean; Fanning, Lev T. D.; Sheth, Urvi; Martinborough, Esther; Termin, Andreas; Neubert, Timothy; Zimmermann, Nicole; Knoll, Tara; Whitney, Tara; Kawatkar, Aarti; Lehsten, Danielle; Stamos, Dean; Zhou, Jinglan; Arumugam, Vijayalaksmi; Gutierrez, Corey

PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 369pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

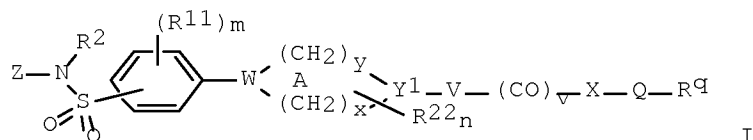
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007075895	A2	20070705	WO 2006-US48802	20061221
WO 2007075895	A3	20071129		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
US 20080027067	A1	20080131	US 2006-643622	20061221

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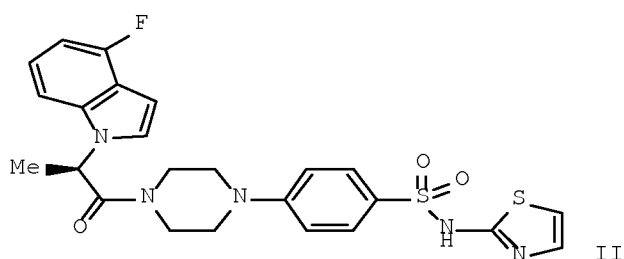
PRIORITY APPLN. INFO.:

US 2005-752926P	P	20051221
US 2006-791181P	P	20060411
US 2006-799797P	P	20060512
US 2006-839444P	P	20060823

OTHER SOURCE(S): MARPAT 147:143468
GI



I



II

AB The invention relates to heterocyclic derivs. of formula I useful as inhibitors of ion channels. Compound of formula I wherein Z is (un)substituted 5- to 7-membered (un)saturated heterocycle; W and Y1 are independently CH and H, provided that at least one of W and Y1 is N; x and y are independently 0 - 3, provided that x + y is 2, 3 and 4; m and n are independently 0 - 4; v is 0 and 1; Q is a bond, (un)branched (un)functionalized C1-6 alkylidene; Rq is (un)substituted C1-6 aliphatic, (un)substituted 3 to 8-membered (un)saturated mono(hetero)cycle, and (un)substituted 8- to 15-membered (un)saturated (bi/tri/spiro)(hetero)cycle; R11 is R2, halo, CN, NO2, CF3, OCF3, OH, etc.; R22 is R2, =O, =NNH2 and derivs., =N-OH and derivs., OH and derivs., O-acyl, OCO2H and derivs., etc.; R2 is H, (un)substituted C1-6 aliphatic; ring A may be optionally fused with (un)substituted phenyl; and their pharmaceutically acceptable salts thereof, are claimed. The invention also provides pharmaceutically acceptable compns. comprising the compds. of the invention and methods of using the compns. in the treatment of various disorders. Compound II was prepared by acylation of 4-(piperazin-1-yl)-N-(thiazol-2-yl)benzenesulfonamide with (2R)-2-(fluoroindol-1-yl)propionic acid. All the invention compds. were evaluated for their sodium channel inhibitory activity.

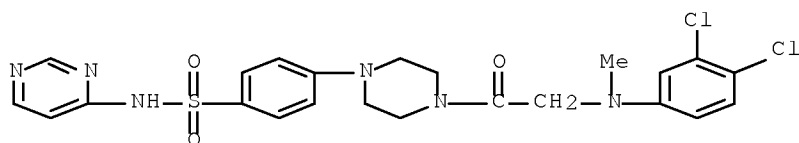
IT 943645-09-8P 943645-63-4P 943652-50-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of heterocyclic derivs. as inhibitors of ion channels useful in treatment of various disorders)

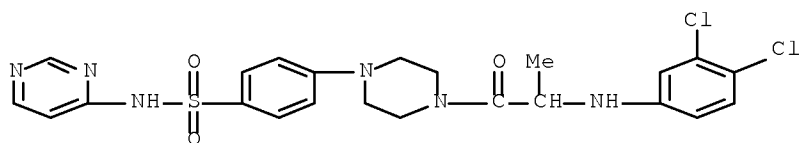
RN 943645-09-8 ZCAPLUS

CN Benzenesulfonamide, 4-[4-[2-[(3,4-dichlorophenyl)methylamino]acetyl]-1-piperazinyl]-N-4-pyrimidinyl- (CA INDEX NAME)



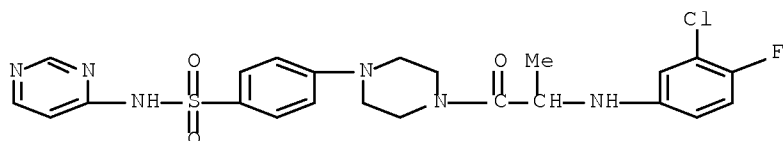
RN 943645-63-4 ZCAPLUS

CN Benzenesulfonamide, 4-[4-[2-[(3,4-dichlorophenyl)amino]-1-oxopropyl]-1-piperazinyl]-N-4-pyrimidinyl- (CA INDEX NAME)



RN 943652-50-4 ZCAPLUS

CN Benzenesulfonamide, 4-[4-[2-[(3-chloro-4-fluorophenyl)amino]-1-oxopropyl]-1-piperazinyl]-N-4-pyrimidinyl- (CA INDEX NAME)



L58 ANSWER 5 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:31168 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 146:142515

TITLE: Quinolinones, chromenones, benzothiopyranones, and anilines as androgen receptor modulators, their preparation, pharmaceutical compositions, and use in therapy

INVENTOR(S): Loren, Jon C.; Miller, Todd; Pedram, Bijan; Rowley, Charlene V.; Shen, Yixing; Van Oeveren, Cornelis A.; Zhi, Lin

PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 278pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2007005887 A2 20070111 WO 2006-US26067 20060630
 WO 2007005887 A3 20070419

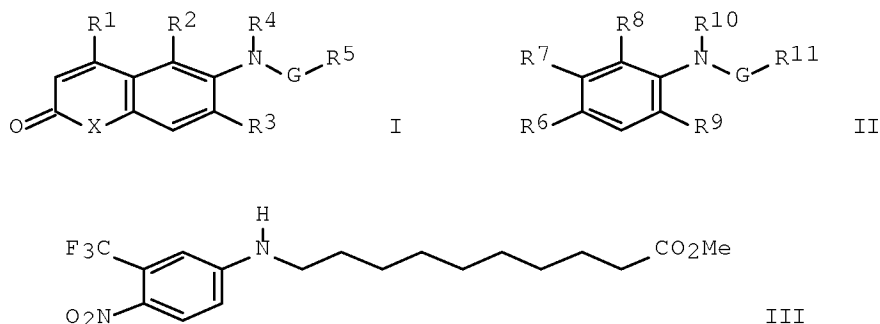
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-695949P P 20050701

OTHER SOURCE(S): MARPAT 146:142515

GI



AB The invention relates to compds. of general formulas I, II or related derivs., which are androgen receptor modulators. In compds. I, X is O, S, or (un)substituted N; G is a bond, C(O), C(S), or S(O)₂; R₁, R₂, and R₃ are independently selected from H, halo, OH, SH, NH₂, C1-6 alkoxy, C1-6 haloalkoxy, C1-6 alkylthio, C1-6 alkylamino, (un)substituted C1-4 alkyl, (un)substituted C1-4 haloalkyl, etc.; and R₄ and R₅ are independently selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, etc.; including pharmaceutically acceptable salts and prodrugs thereof. In compds. II, G is as defined previously; R₆ and R₇ are independently selected from halo, cyano, nitro, C1-4 alkyl, C1-4 haloalkyl, C1-4 heteroalkyl, and C1-4 heterohaloalkyl; R₈ and R₉ are independently selected from H, halo, OH, SH, NH₂, C1-6 alkoxy, C1-6 haloalkoxy, C1-6 alkylthio, C1-6 alkylamino, (un)substituted C1-4 alkyl, (un)substituted C1-4 haloalkyl, (un)substituted C1-4 heteroalkyl, etc.; and R₁₀ and R₁₁ are independently selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, etc.; including pharmaceutically acceptable salts and prodrugs thereof. The invention also relates to the preparation of the compds. of the invention, pharmaceutical compns. comprising a compound of the invention and a pharmaceutically acceptable carrier, as well as to the use of the compns. for the treatment or prevention of conditions that respond to androgen receptor modulation, such as acne, male-pattern baldness, infertility, and impotence.

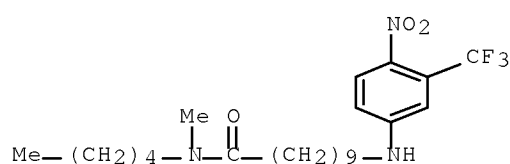
10/598508

Substitution of Me 10-bromodecanoate with 4-nitro-3-trifluoromethylaniline gave aminodecanoate III. Some compds. of the invention are agonists of androgen receptors, but other compds. are antagonists of androgen receptors (no data).

IT 918893-50-2P, 10-(4-Nitro-3-trifluoromethylphenylamino)decanoic acid N-methyl-N-pentylamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of quinolinones, chromenones, benzothiopyranones, and anilines for use as androgen receptor modulators)

RN 918893-50-2 ZCAPLUS

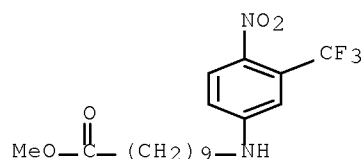
CN Decanamide, N-methyl-10-[[4-nitro-3-(trifluoromethyl)phenyl]amino]-N-pentyl- (CA INDEX NAME)



IT 918893-47-7P, 10-(4-Nitro-3-trifluoromethylphenylamino)decanoic acid methyl ester 918893-49-9P, 10-(4-Nitro-3-trifluoromethylphenylamino)decanoic acid 918893-52-4P, 10-(4-Nitro-3-trifluoromethylphenylamino)-1-piperidin-1-yldecan-1-one 918893-61-5P, 10-[(4-Nitro-3-trifluoromethylphenyl)(2,2,2-trifluoroethyl)amino]decanoic acid N-methyl-N-pentylamide 918893-62-6P, 10-[N-(4-Nitro-3-trifluoromethylphenyl)-N-(2,2,2-trifluoroethyl)amino]-1-piperidin-1-yldecan-1-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of quinolinones, chromenones, benzothiopyranones, and anilines for use as androgen receptor modulators)

RN 918893-47-7 ZCAPLUS

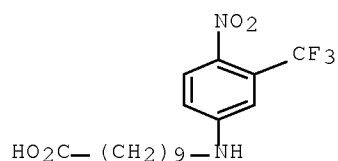
CN Decanoic acid, 10-[[4-nitro-3-(trifluoromethyl)phenyl]amino]-, methyl ester (CA INDEX NAME)



RN 918893-49-9 ZCAPLUS

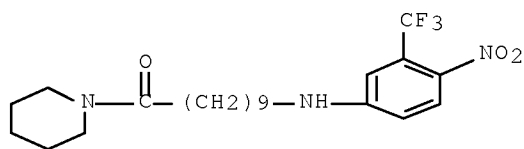
CN Decanoic acid, 10-[[4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

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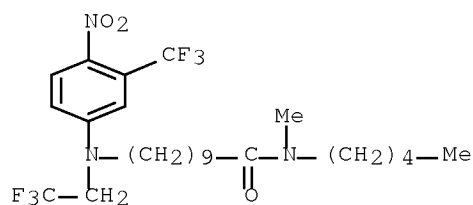
RN 918893-52-4 ZCAPLUS

CN 1-Decanone, 10-[[4-nitro-3-(trifluoromethyl)phenyl]amino]-1-(1-piperidinyl)- (CA INDEX NAME)



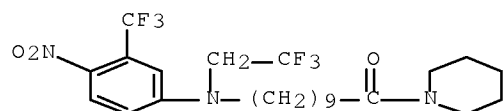
RN 918893-61-5 ZCAPLUS

CN Decanamide, N-methyl-10-[[4-nitro-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-pentyl- (CA INDEX NAME)



RN 918893-62-6 ZCAPLUS

CN 1-Decanone, 10-[[4-nitro-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-1-(1-piperidinyl)- (CA INDEX NAME)



L58 ANSWER 6 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1343064 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 146:287642

TITLE: Design and Synthesis of an Array of Selective Androgen Receptor Modulators

10/598508

AUTHOR(S): Trump, Ryan P.; Blanc, Jean-Baptiste E.; Stewart, Eugene L.; Brown, Peter J.; Caivano, Matilde; Gray, David W.; Hoekstra, William J.; Willson, Timothy M.; Han, Bajin; Turnbull, Philip

CORPORATE SOURCE: GlaxoSmithKline, Research Triangle Park, NC, 27709, USA

SOURCE: Journal of Combinatorial Chemistry (2007), 9(1), 107-114
CODEN: JCCHFF; ISSN: 1520-4766

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe the design, using shape comparison and fast docking computer algorithms, and rapid parallel synthesis of a 1300 member array based on GSK7721, a 4-aminobenzonitrile androgen receptor (AR) antagonist identified by focused screening of the GSK compound collection. The array yielded 352 submicromolar and 17 subnanomolar AR agonists as measured by a cell-based reporter gene functional assay. The rapid synthesis of a large number of active compds. provided valuable information in the optimization of AR modulators, which may be useful in treating androgen deficiency in aging males.

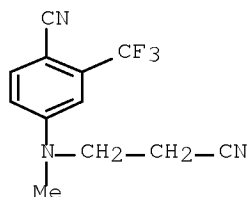
IT 864284-72-0P 927692-51-1P 927692-77-1P
927693-09-2P 927693-34-3P 927693-70-7P
927693-96-7P 927694-28-8P 927694-51-7P
927695-05-4P 927695-39-4P 927695-65-6P
927698-87-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Design and Synthesis of an Array of Selective Androgen Receptor Modulators)

RN 864284-72-0 ZCAPLUS

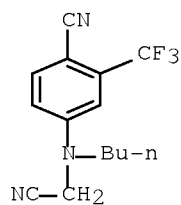
CN Benzonitrile, 4-[(2-cyanoethyl)methylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 927692-51-1 ZCAPLUS

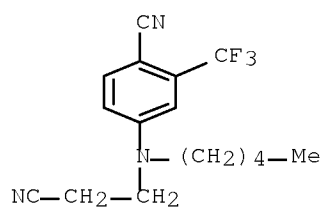
CN Benzonitrile, 4-[butyl(cyanomethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

10/598508



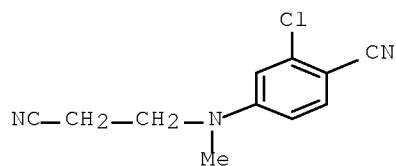
RN 927692-77-1 ZCAPLUS

CN Benzonitrile, 4-[(2-cyanoethyl)pentylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



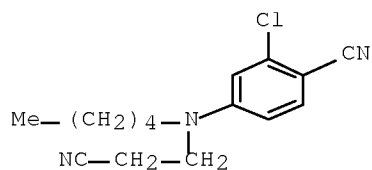
RN 927693-09-2 ZCAPLUS

CN Benzonitrile, 2-chloro-4-[(2-cyanoethyl)methylamino]- (CA INDEX NAME)



RN 927693-34-3 ZCAPLUS

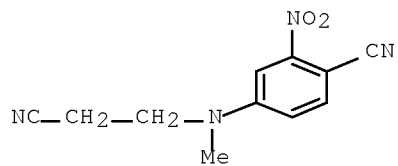
CN Benzonitrile, 2-chloro-4-[(2-cyanoethyl)pentylamino]- (CA INDEX NAME)



RN 927693-70-7 ZCAPLUS

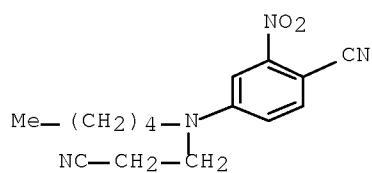
CN Benzonitrile, 4-[(2-cyanoethyl)methylamino]-2-nitro- (CA INDEX NAME)

10/598508



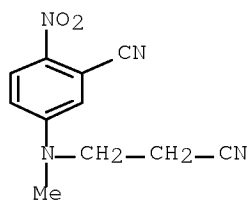
RN 927693-96-7 ZCAPLUS

CN Benzonitrile, 4-[(2-cyanoethyl)pentylamino]-2-nitro- (CA INDEX NAME)



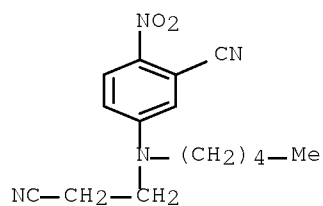
RN 927694-28-8 ZCAPLUS

CN Benzonitrile, 5-[(2-cyanoethyl)methylamino]-2-nitro- (CA INDEX NAME)



RN 927694-51-7 ZCAPLUS

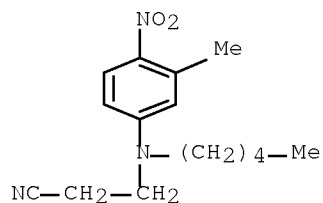
CN Benzonitrile, 5-[(2-cyanoethyl)pentylamino]-2-nitro- (CA INDEX NAME)



RN 927695-05-4 ZCAPLUS

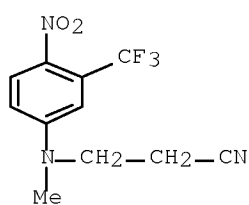
CN Propanenitrile, 3-[(3-methyl-4-nitrophenyl)pentylamino]- (CA INDEX NAME)

10/598508



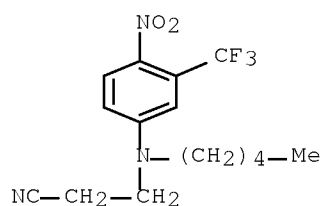
RN 927695-39-4 ZCAPLUS

CN Propanenitrile, 3-[methyl[4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



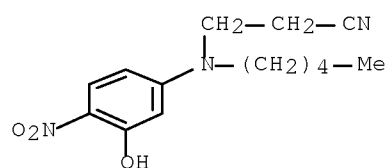
RN 927695-65-6 ZCAPLUS

CN Propanenitrile, 3-[[4-nitro-3-(trifluoromethyl)phenyl]pentylamino]- (CA INDEX NAME)



RN 927698-87-1 ZCAPLUS

CN Propanenitrile, 3-[(3-hydroxy-4-nitrophenyl)pentylamino]- (CA INDEX NAME)



10/598508

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 7 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1312622 ZCAPLUS Full-text

DOCUMENT NUMBER: 146:62449

TITLE: Nonsteroidal tertiary arylamines as modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors and their preparation and use for treatment of diseases

INVENTOR(S): Turnbull, Philip Stewart; Cadilla, Rodolfo; Larkin, Andrew Lamont; Stewart, Eugene Lee; Stetson, Katherine

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 191pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

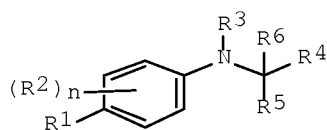
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

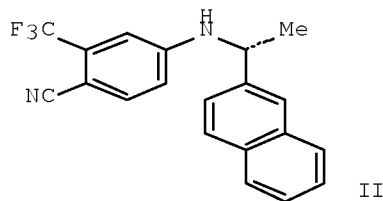
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006133216	A2	20061214	WO 2006-US21966	20060606
WO 2006133216	A3	20070426		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
EP 1888512	A2	20080220	EP 2006-772327	20060606
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR				
PRIORITY APPLN. INFO.:			US 2005-687895P	P 20050606
			WO 2006-US21966	W 20060606

OTHER SOURCE(S): MARPAT 146:62449

GI



I



II

AB This invention relates to non-steroidal compds. of formula I that are modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, and also to the methods for the making and use of such compds. Compds. of formula I wherein R1 is CN, NO2 and halo; n is 0, 1, and 2; each R3 is independently CN, NO2, halo, (halo)alkyl, alkenyl, alkynyl, OH, (halo)alkoxy, and aryl; R3 is (Rx)aR7; Rx is (un)substituted C1-4 alkylene; a is 0 and 1; R7 is H, (halo)alkyl, cycloalkyl, alkenyl, alkynyl, CN; R4 and R5 are independently H, (halo)alkyl, and cycloalkyl; R6 is (un)substituted aryl and (un)substituted heterocyclyl; and their pharmaceutically acceptable salts, and solvates thereof are claimed. Example compound II was prepared by substitution of 4-fluoro-2-trifluoromethylbenzonitrile with (R)-(+)-1-(2-naphthyl)ethylamine; the resulting 4-[[1-(2-naphthyl)ethyl]amino]-2-trifluoromethylbenzonitrile underwent N-alkylation with cyclopropanemethyl bromide to give compound II. All the invention compds. were evaluated for their androgen, glucocorticoid, mineralocorticoid, and progesterone receptor modulatory activity. From the assay, it was determined that some of the compds. exhibited pIC50 values of ≥ 5.0 .

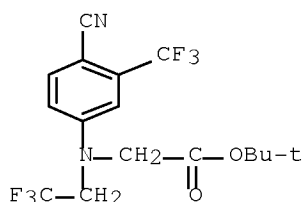
IT 864283-46-5P 864283-47-6P 864283-48-7P
864284-35-5P 864284-74-2P 864284-76-4P
864285-03-0P 864285-05-2P 864285-65-4P
864285-67-6P 916810-72-5P 916810-76-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of nonsteroidal tertiary arylamines as modulators of androgen, glucocorticoid, mineralocorticoid and progesterone receptors useful in therapy)

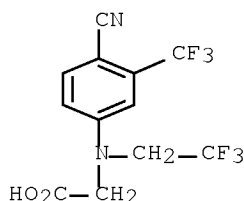
RN 864283-46-5 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864283-47-6 ZCAPLUS

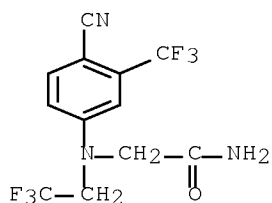
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



10/598508

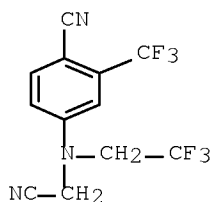
RN 864283-48-7 ZCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



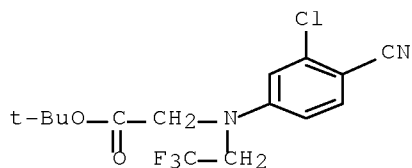
RN 864284-35-5 ZCAPLUS

CN Benzonitrile, 4-[(cyanomethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 864284-74-2 ZCAPLUS

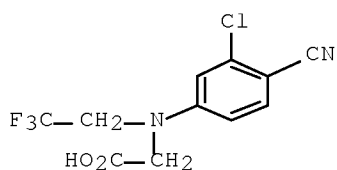
CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864284-76-4 ZCAPLUS

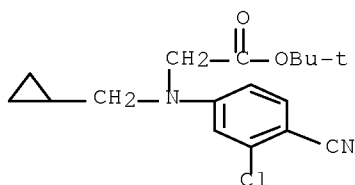
CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

10/598508



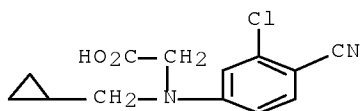
RN 864285-03-0 ZCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)-,
1,1-dimethylethyl ester (CA INDEX NAME)



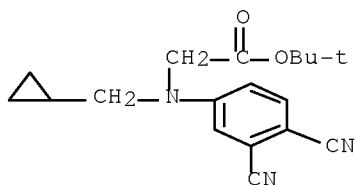
RN 864285-05-2 ZCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)- (CA INDEX
NAME)



RN 864285-65-4 ZCAPLUS

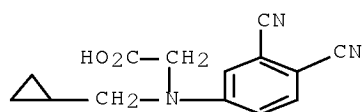
CN Glycine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)-, 1,1-dimethylethyl
ester (CA INDEX NAME)



RN 864285-67-6 ZCAPLUS

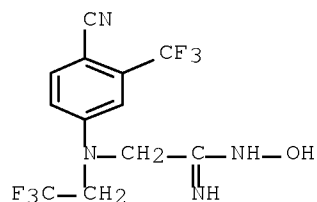
CN Glycine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)- (CA INDEX NAME)

10/598508



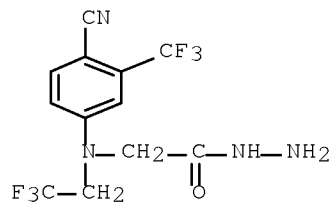
RN 916810-72-5 ZCAPLUS

CN Ethanimidamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-hydroxy- (CA INDEX NAME)



RN 916810-76-9 ZCAPLUS

CN Acetic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-, hydrazide (CA INDEX NAME)



L58 ANSWER 8 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1207137 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:500021

TITLE: Antineoplastic compounds and pharmaceutical compositions containing same

INVENTOR(S): Rodriguez Fernandez, Rolando Eduardo; Vera Alvarez, Roberto; De la Nuez Veulens, Ania; Mazola Reyes, Yuliet; Perea Rodriguez, Silvio Ernesto; Acevedo Castro, Boris Ernesto; Musacchio Lasa, Alexis; Ubieta Gomez, Raimundo

PATENT ASSIGNEE(S): Centro de Ingenieria Genetica y Biotecnologia, Cuba

SOURCE: PCT Int. Appl., 24pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Spanish

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

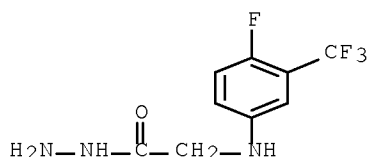
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006119713	A2	20061116	WO 2006-CU2	20060505
WO 2006119713	A3	20070301		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006246204	A1	20061116	AU 2006-246204	20060505
CA 2607298	A1	20061116	CA 2006-2607298	20060505
EP 1892245	A2	20080227	EP 2006-753157	20060505
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
MX 200714216	A	20080207	MX 2007-14216	20071112
KR 2008008407	A	20080123	KR 2007-728594	20071207
PRIORITY APPLN. INFO.:			CU 2005-91	A 20050512
			WO 2006-CU2	W 20060505

AB The invention relates to chemical compds. which are obtained by means of in silico mol. modeling and which have a structure that can be used to block phosphorylation by interacting said compds. with the phosphorylation domain or the environment thereof in the substrates of casein kinase II enzyme. The invention also relates to pharmaceutical compns. that contain said compds. and to the use thereof in the preparation of medicaments for the treatment of diseases associated with neoplastic processes. Compds. of the invention demonstrated antitumor activity against non-small cell lung cancer in a rat model.

IT 501008-37-3
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (antineoplastic compds. and pharmaceutical compns. containing same)

RN 501008-37-3 ZCAPLUS

CN Glycine, N-[4-fluoro-3-(trifluoromethyl)phenyl]-, hydrazide (CA INDEX NAME)

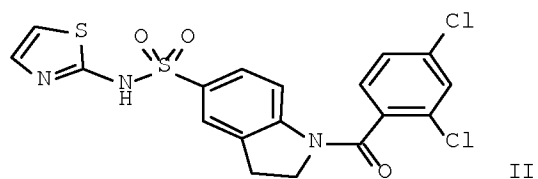
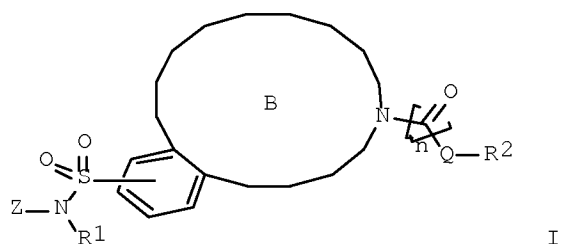


L58 ANSWER 9 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:1206349 ZCAPLUS Full-text
 DOCUMENT NUMBER: 145:505437
 TITLE: Thiazolyl azabicyclesulfonamide derivatives as modulators of ion channels and their preparation, pharmaceutical composition and their use in the

10/598508

INVENTOR(S): treatment of various conditions
Kawatkar, Aarti S.; Whitney, Tara; Neubert, Timothy
D.; Zimmermann, Nicole; Termin, Andreas P.;
Martinborough, Esther
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 132pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006122014	A2	20061116	WO 2006-US17699	20060508
WO 2006122014	A3	20061228		
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006244206	A1	20061116	AU 2006-244206	20060508
CA 2607670	A1	20061116	CA 2006-2607670	20060508
EP 1891063	A2	20080227	EP 2006-752393	20060508
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
MX 200714180	A	20080114	MX 2007-14180	20071112
IN 2007KN04385	A	20080509	IN 2007-KN4385	20071115
NO 2007006306	A	20071207	NO 2007-6306	20071207
KR 2008015102	A	20080218	KR 2007-728820	20071210
PRIORITY APPLN. INFO.:			US 2005-679691P	P 20050510
			WO 2006-US17699	W 20060508
OTHER SOURCE(S):			MARPAT 145:505437	
GI				



AB Bicyclic derivs. having formula I and a composition thereof are useful as ion channel antagonists. Compds. of formula I wherein Z is (un)substituted 5- to 7-membered unsatd. or aromatic ring having at least one heteroatom; ring B is (un)substituted 5- to 7-membered monocyclic unsatd. or aromatic ring with at least one heteroatom; Q is a bond, (un)substituted C1-6 (un)branched alkylidene; R1 is H and (un)substituted C1-6 aliphatic; R2 is C1-6 aliphatic, 3- to 8-membered (un)saturated (hetero)monocycle, (un)saturated 8- to 12-membered (hetero)bicycle; q is 0 and 1; and their pharmaceutically acceptable salts are claimed. Example compound II was prepared by N-acylation of. N-(thiazol-2-yl) 5-indolinesulfonamide with 2,4-dichlorobenzoic acid. All the invention compds. were evaluated for their sodium channel inhibitory activity. Some of the invention compds. exhibited IC50 values of < 2 μ M.

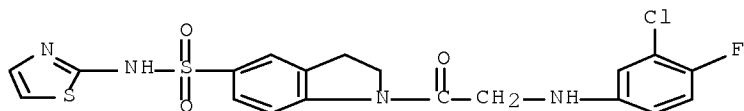
IT 914920-52-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of thiazolyl azabicyclesulfonamide derivs. as modulators of ion channels)

RN 914920-52-8 ZCAPLUS

CN 1H-Indole-5-sulfonamide, 1-[2-[(3-chloro-4-fluorophenyl)amino]acetyl]-2,3-dihydro-N-2-thiazolyl- (CA INDEX NAME)



L58 ANSWER 10 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1122964 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:455269

TITLE: Preparation of N-cyanoaryl amino acid amides for treating endometriosis or uterine fibroids

10/598508

INVENTOR(S): Jones, David G.; Kaldor, Istvan; Liang, Xi; Turnbull, Philip Stewart; Hammond, Marlys; Kallander, Lara S.; Thompson, Scott Kevin; Washburn, David
 PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA
 SOURCE: PCT Int. Appl., 71pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006113552	A2	20061026	WO 2006-US14286	20060414
WO 2006113552	A3	20070531		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA EP 1871379 A2 20080102 EP 2006-750349 20060414 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU PRIORITY APPLN. INFO.: US 2005-671592P P 20050415 WO 2006-US14286 W 20060414				

OTHER SOURCE(S): MARPAT 145:455269

AB The invention relates to amino acid amides NC-Ar-N(CHR1R1')CR2R2'CONR3R3' [Ar is Ph or naphthyl which may be further substituted; R1, R1' are independently H, (un)substituted alkyl, cycloalkyl, aryl, heteroaryl, or together form a cycloalkyl or cycloalkenyl group; R2, R2' are independently H, (un)substituted alkyl, cycloalkyl, or R4(CH2)m-X-, where R4 is cycloalkyl, Ph, or pyridyl, m is 0-4, and X is a bond, O, or S; R3, R3' are independently (un)substituted alkyl, alkenyl, propargyl; or NR3R3' is heterocycloalkyl (with provisos)] or their pharmaceutically-acceptable salts and their use for treating endometriosis or uterine fibroids. Thus, N2-[(2-chlorophenyl)methyl]-N2-[4-cyano-3-(trifluoromethyl)phenyl]-N1,N1- dimethyl-L-alaninamide was prepared via amidation, arylation, and alkylation reactions. One hundred twenty-two synthesized compds. showed IC50 < 10 µM in the PR binding assay.

IT 913287-47-5P 913287-53-3P 913287-58-8P

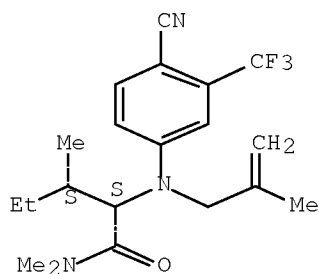
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of N-cyanoaryl amino acid amides for treating endometriosis or uterine fibroids)

RN 913287-47-5 ZCAPLUS

CN Pentanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2-methyl-2-propen-1-yl)amino]-N,N,3-trimethyl-, (2S,3S)- (CA INDEX NAME)

Absolute stereochemistry.

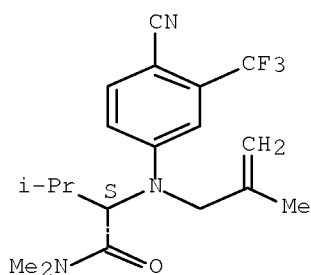
10/598508



RN 913287-53-3 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2-methyl-2-propen-1-yl)amino]-N,N,3-trimethyl-, (2S)- (CA INDEX NAME)

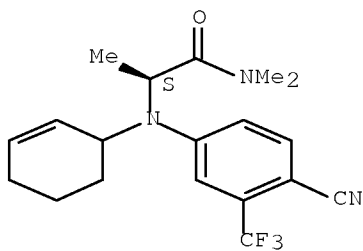
Absolute stereochemistry.



RN 913287-58-8 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]-2-cyclohexen-1-ylamino]-N,N-dimethyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 913287-45-3P 913287-48-6P 913287-50-0P
913287-56-6P 913287-59-9P 913287-71-5P
913287-76-0P 913287-77-1P 913287-78-2P
913287-79-3P 913288-02-5P 913288-03-6P
913288-04-7P 913288-05-8P 913288-06-9P
913288-07-0P 913288-08-1P 913288-09-2P
913288-10-5P 913288-11-6P 913288-12-7P
913288-13-8P 913288-14-9P 913288-15-0P

10/598508

913288-19-4P 913288-20-7P 913288-21-8P
913288-23-0P 913288-25-2P 913288-26-3P
913288-27-4P 913288-28-5P 913288-29-6P
913288-30-9P 913288-31-0P 913288-32-1P
913288-33-2P 913288-34-3P 913288-35-4P
913288-36-5P 913288-37-6P 913288-38-7P
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913288-45-6P 913288-46-7P 913288-47-8P
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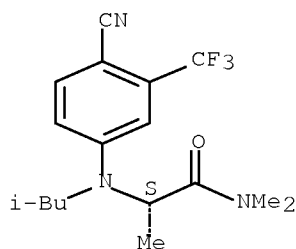
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of N-cyanoaryl amino acid amides for treating endometriosis or
uterine fibroids)

RN 913287-45-3 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2-methylpropyl)amino]-
N,N-dimethyl-, (2S)- (CA INDEX NAME)

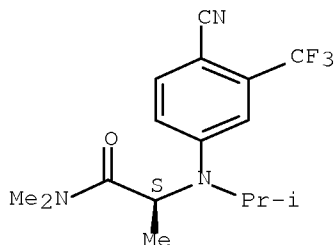
Absolute stereochemistry.



RN 913287-48-6 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](1-methylethyl)amino]-
N,N-dimethyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

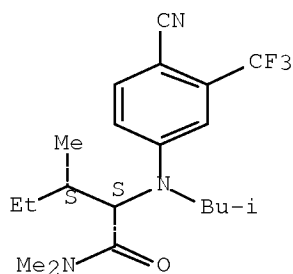


RN 913287-50-0 ZCAPLUS

CN Pentanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2-methylpropyl)amino]-
N,N,3-trimethyl-, (2S,3S)- (CA INDEX NAME)

Absolute stereochemistry.

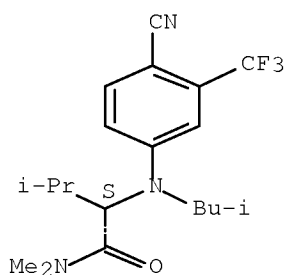
10/598508



RN 913287-56-6 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2-methylpropyl)amino]-N,N,3-trimethyl-, (2S)- (CA INDEX NAME)

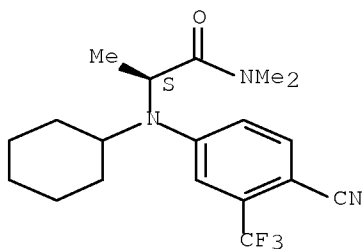
Absolute stereochemistry.



RN 913287-59-9 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]cyclohexylamino]-N,N-dimethyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

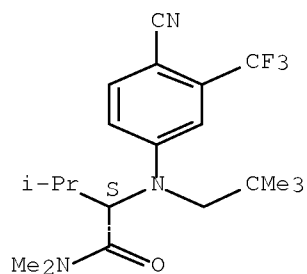


RN 913287-71-5 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2-dimethylpropyl)amino]-N,N,3-trimethyl-, (2S)- (CA INDEX NAME)

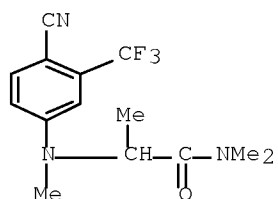
Absolute stereochemistry.

10/598508



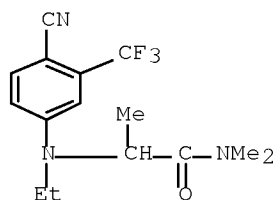
RN 913287-76-0 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]methylamino]-N,N-dimethyl- (CA INDEX NAME)



RN 913287-77-1 ZCAPLUS

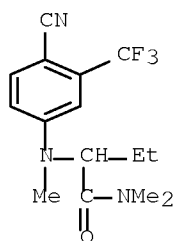
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]ethylamino]-N,N-dimethyl- (CA INDEX NAME)



RN 913287-78-2 ZCAPLUS

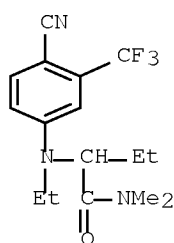
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]methylamino]-N,N-dimethyl- (CA INDEX NAME)

10/598508



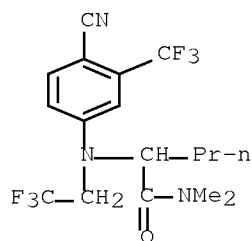
RN 913287-79-3 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]ethylamino]-N,N-dimethyl-
(CA INDEX NAME)



RN 913288-02-5 ZCAPLUS

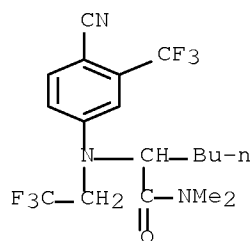
CN Pentanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)



RN 913288-03-6 ZCAPLUS

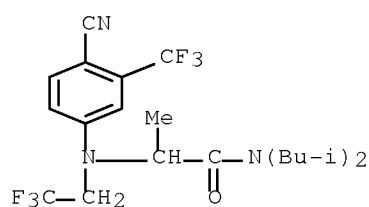
CN Hexanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)

10/598508



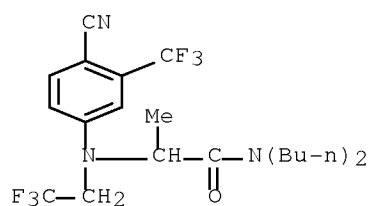
RN 913288-04-7 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]-(2,2,2-trifluoroethyl)amino]-N,N-bis(2-methylpropyl)- (CA INDEX NAME)



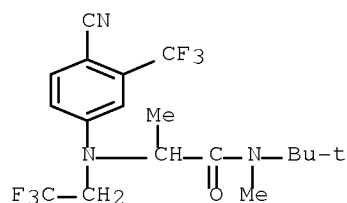
RN 913288-05-8 ZCAPLUS

CN Propanamide, N,N-dibutyl-2-[[4-cyano-3-(trifluoromethyl)phenyl]-(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



RN 913288-06-9 ZCAPLUS

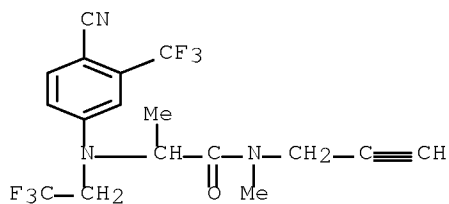
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]-(2,2,2-trifluoroethyl)amino]-N-(1,1-dimethylethyl)-N-methyl- (CA INDEX NAME)



10/598508

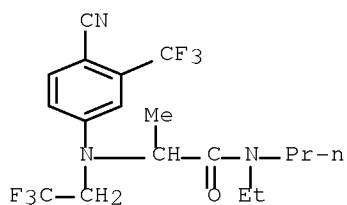
RN 913288-07-0 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-2-propyn-1-yl- (CA INDEX NAME)



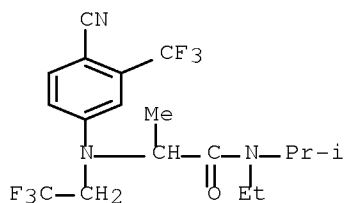
RN 913288-08-1 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-propyl- (CA INDEX NAME)



RN 913288-09-2 ZCAPLUS

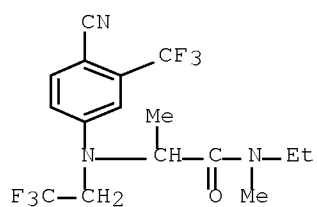
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-(1-methylethyl)- (CA INDEX NAME)



RN 913288-10-5 ZCAPLUS

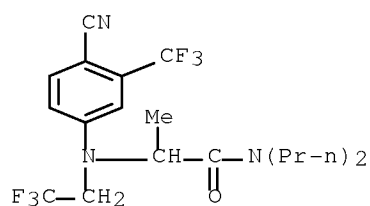
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-methyl- (CA INDEX NAME)

10/598508



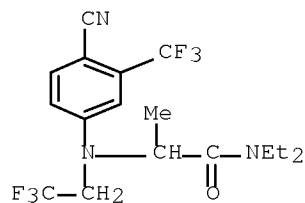
RN 913288-11-6 ZCAPLUS

CN Propanamide, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dipropyl- (CA INDEX NAME)



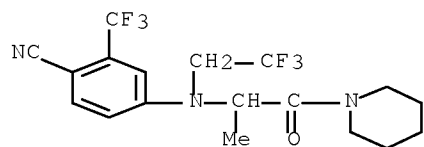
RN 913288-12-7 ZCAPLUS

CN Propanamide, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-diethyl- (CA INDEX NAME)



RN 913288-13-8 ZCAPLUS

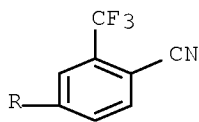
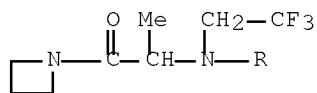
CN Benzonitrile, 4-[[[1-methyl-2-oxo-2-(1-piperidinyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 913288-14-9 ZCAPLUS

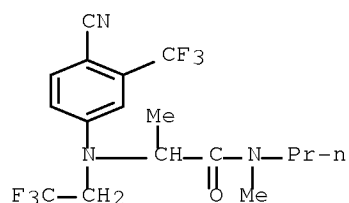
10/598508

CN Benzonitrile, 4-[[2-(1-azetidiny1)-1-methyl-2-oxoethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



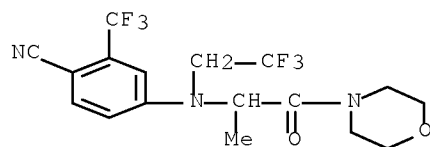
RN 913288-15-0 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-propyl- (CA INDEX NAME)



RN 913288-19-4 ZCAPLUS

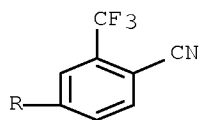
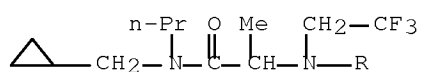
CN Benzonitrile, 4-[[1-methyl-2-(4-morpholinyl)-2-oxoethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 913288-20-7 ZCAPLUS

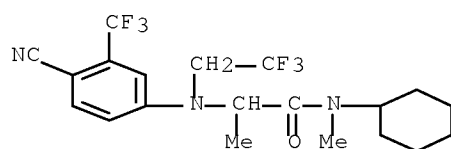
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(cyclopropylmethyl)-N-propyl- (CA INDEX NAME)

10/598508



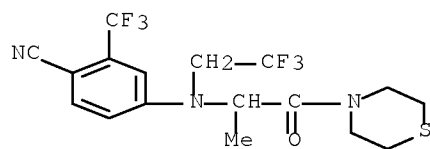
RN 913288-21-8 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-cyclohexyl-N-methyl- (CA INDEX NAME)



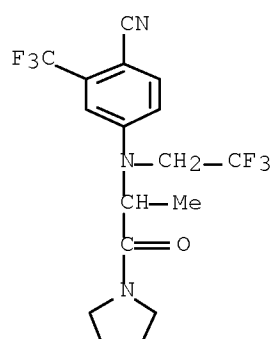
RN 913288-23-0 ZCAPLUS

CN Benzonitrile, 4-[[1-methyl-2-oxo-2-(4-thiomorpholinyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 913288-25-2 ZCAPLUS

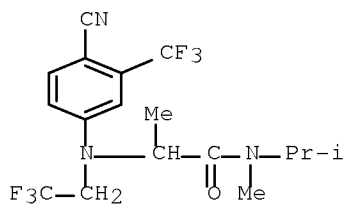
CN Benzonitrile, 4-[[1-methyl-2-oxo-2-(1-pyrrolidinyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



10/598508

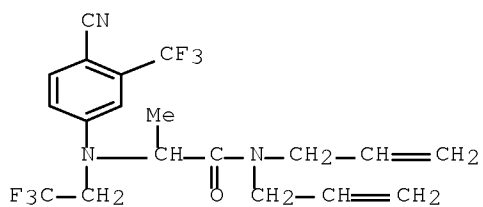
RN 913288-26-3 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-(1-methylethyl)- (CA INDEX NAME)



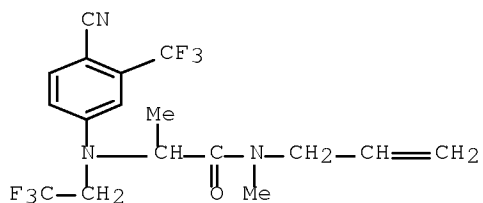
RN 913288-27-4 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-di-2-propen-1-yl- (CA INDEX NAME)



RN 913288-28-5 ZCAPLUS

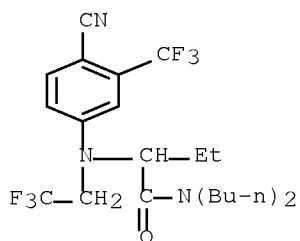
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-2-propen-1-yl- (CA INDEX NAME)



RN 913288-29-6 ZCAPLUS

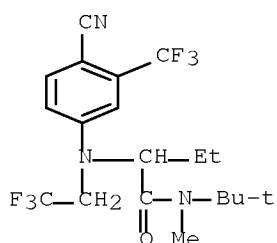
CN Butanamide, N,N-dibutyl-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

10/598508



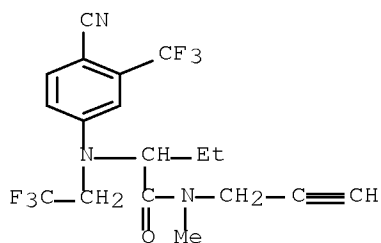
RN 913288-30-9 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(1,1-dimethylethyl)-N-methyl- (CA INDEX NAME)



RN 913288-31-0 ZCAPLUS

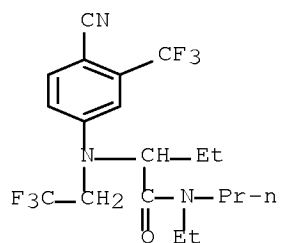
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-2-propyn-1-yl- (CA INDEX NAME)



RN 913288-32-1 ZCAPLUS

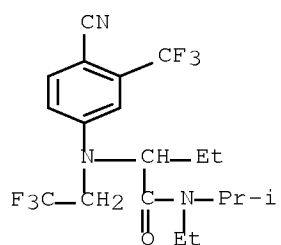
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-propyl- (CA INDEX NAME)

10/598508



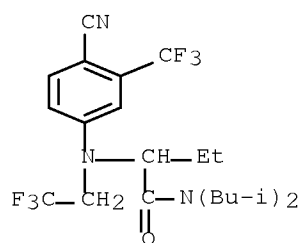
RN 913288-33-2 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-(1-methylethyl)- (CA INDEX NAME)



RN 913288-34-3 ZCAPLUS

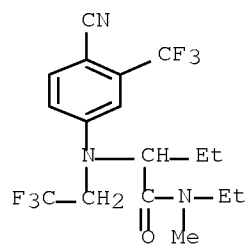
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-bis(2-methylpropyl)- (CA INDEX NAME)



RN 913288-35-4 ZCAPLUS

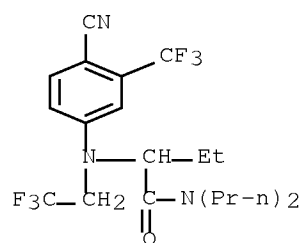
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-methyl- (CA INDEX NAME)

10/598508



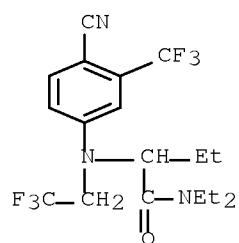
RN 913288-36-5 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dipropyl- (CA INDEX NAME)



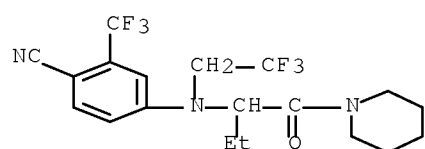
RN 913288-37-6 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-diethyl- (CA INDEX NAME)



RN 913288-38-7 ZCAPLUS

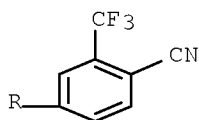
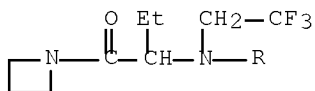
CN Benzonitrile, 4-[[1-(1-piperidinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



10/598508

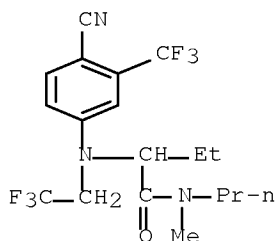
RN 913288-39-8 ZCAPLUS

CN Benzonitrile, 4-[[1-(1-azetidinyldicarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



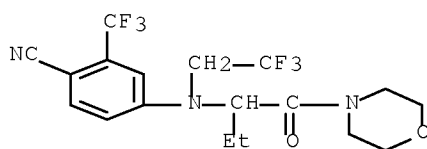
RN 913288-40-1 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-propyl- (CA INDEX NAME)



RN 913288-44-5 ZCAPLUS

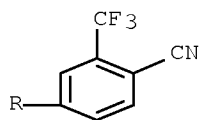
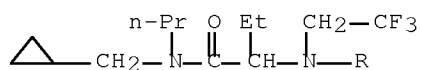
CN Benzonitrile, 4-[[1-(4-morpholinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 913288-45-6 ZCAPLUS

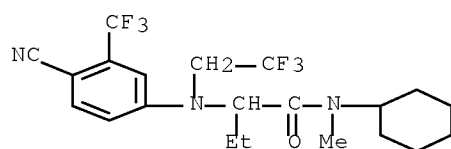
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(cyclopropylmethyl)-N-propyl- (CA INDEX NAME)

10/598508



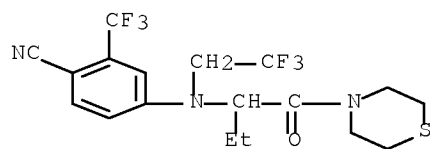
RN 913288-46-7 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-cyclohexyl-N-methyl- (CA INDEX NAME)



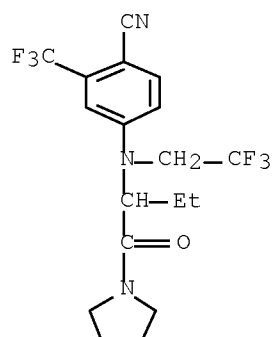
RN 913288-47-8 ZCAPLUS

CN Benzonitrile, 4-[[1-(4-thiomorpholinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 913288-50-3 ZCAPLUS

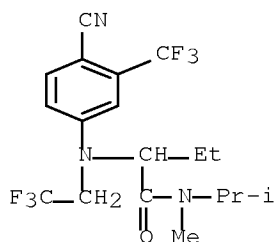
CN Benzonitrile, 4-[[1-(1-pyrrolidinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



10/598508

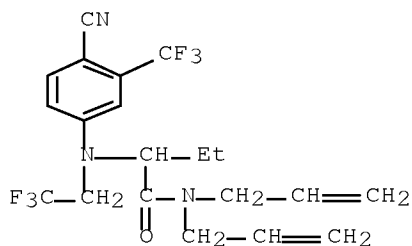
RN 913288-51-4 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-(1-methylethyl)- (CA INDEX NAME)



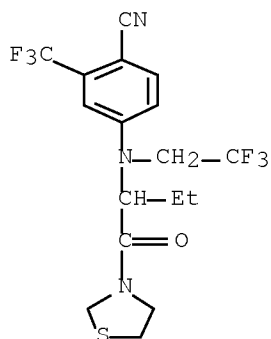
RN 913288-52-5 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-di-2-propen-1-yl- (CA INDEX NAME)



RN 913288-53-6 ZCAPLUS

CN Benzonitrile, 4-[[1-(3-thiazolidinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

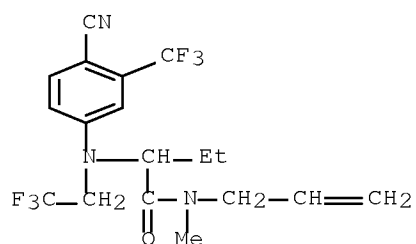


RN 913288-54-7 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-

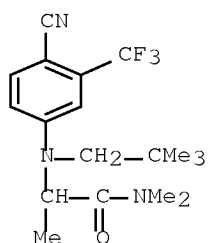
10/598508

trifluoroethyl)amino]-N-methyl-N-2-propen-1-yl- (CA INDEX NAME)



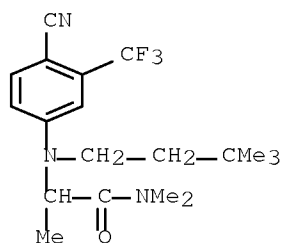
RN 913288-56-9 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2-dimethylpropyl)amino]-N,N-dimethyl- (CA INDEX NAME)



RN 913288-57-0 ZCAPLUS

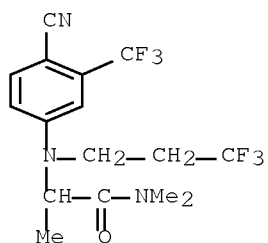
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](3,3-dimethylbutyl)amino]-N,N-dimethyl- (CA INDEX NAME)



RN 913288-58-1 ZCAPLUS

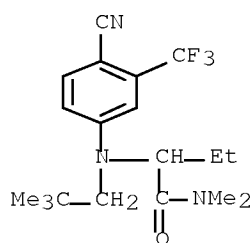
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](3,3,3-trifluoropropyl)amino]-N,N-dimethyl- (CA INDEX NAME)

10/598508



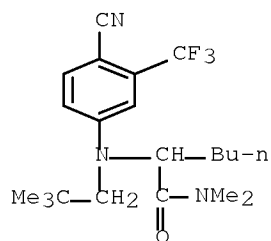
RN 913288-60-5 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2-dimethylpropyl)amino]-N,N-dimethyl- (CA INDEX NAME)



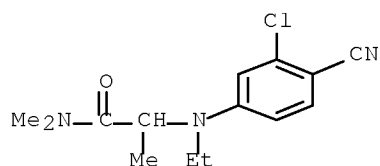
RN 913288-62-7 ZCAPLUS

CN Hexanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2-dimethylpropyl)amino]-N,N-dimethyl- (CA INDEX NAME)



RN 913288-63-8 ZCAPLUS

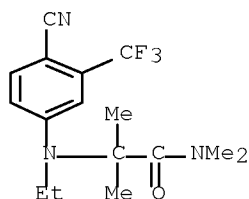
CN Propanamide, 2-[(3-chloro-4-cyanophenyl)ethylamino]-N,N-dimethyl- (CA INDEX NAME)



10/598508

RN 913288-65-0 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]ethylamino]-N,N,2-trimethyl- (CA INDEX NAME)



IT 864283-58-9P 913288-66-1P 913288-69-4P

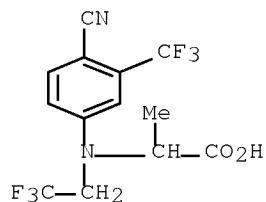
913288-70-7P 913288-72-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-cyanoaryl amino acid amides for treating endometriosis or uterine fibroids)

RN 864283-58-9 ZCAPLUS

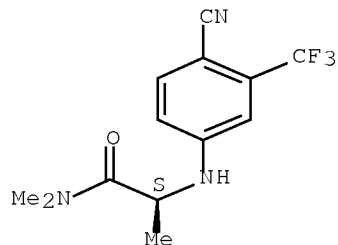
CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



RN 913288-66-1 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]amino]-N,N-dimethyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

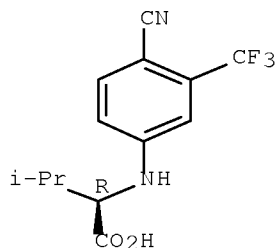


10/598508

RN 913288-69-4 ZCAPLUS

CN D-Valine, N-[4-cyano-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

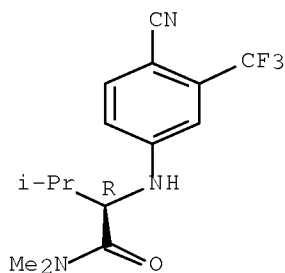
Absolute stereochemistry.



RN 913288-70-7 ZCAPLUS

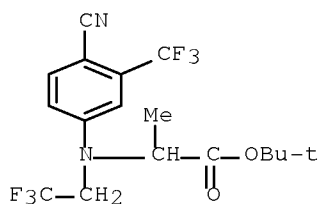
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]amino]-N,N,3-trimethyl-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 913288-72-9 ZCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



L58 ANSWER 11 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:646520 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:314614

TITLE: 2,3-Migration in Rh(II)-Catalyzed Reactions of

β -Trifluoroacetamido α -Diazocarbonyl
Compounds

AUTHOR(S): Xu, Feng; Zhang, Shiwei; Wu, Xiangnan; Liu, Yu; Shi, Weifeng; Wang, Jianbo

CORPORATE SOURCE: Beijing National Laboratory of Molecular Sciences (BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing, 100871, Peop. Rep. China

SOURCE: Organic Letters (2006), 8(15), 3207-3210
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

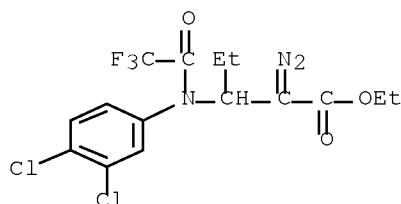
OTHER SOURCE(S): CASREACT 145:314614

AB A hydroxy group was directly converted into the trifluoroacetamido group by reacting β -hydroxy- α -diazo carbonyl compds. with trifluoroacetimidoyl chloride in the presence of DBU. Rhodium(II)-catalyzed reactions of these diazo compds. gave 2,3-migration products in high yields.

IT 909019-70-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of α -trifluoro(imino)ethoxy α, β -unsatd. carboxylic acid esters via rhodium-catalyzed rearrangement reaction of α -diazo- β -(trifluoroacetyl)amino carboxylic acid esters)

RN 909019-70-1 ZCAPLUS

CN Pentanoic acid, 2-diazo-3-[(3,4-dichlorophenyl)(2,2,2-trifluoroacetyl)amino]-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 12 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:529413 ZCAPLUS Full-text

DOCUMENT NUMBER: 145:188833

TITLE: Synthesis and studies on some new fluorine containing triazolothiadiazines as possible antibacterial, antifungal and anticancer agents

AUTHOR(S): Holla, B. Shivarama; Rao, B. Sooryanarayana; Sarojini, B. K.; Akberali, P. M.; Kumari, N. Suchetha

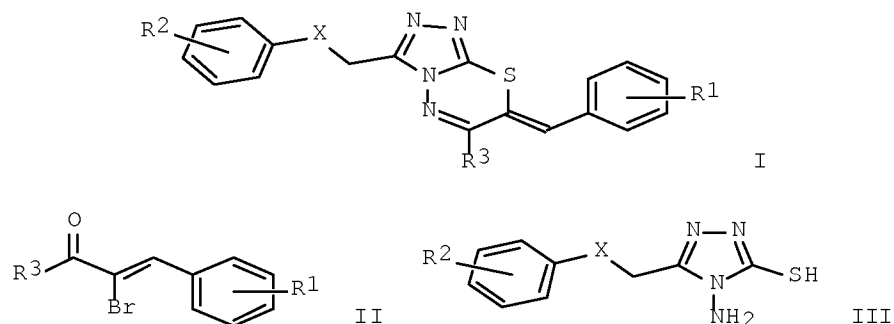
CORPORATE SOURCE: Department of Post-Graduate Studies and Research in Chemistry, Mangalore University, Mangalagangothri, 574 199, India

SOURCE: European Journal of Medicinal Chemistry (2006), 41(5), 657-663
CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier B.V.

10/598508

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 145:188833
 GI



AB A series of 7-arylidene-1,2,4-triazolo[3,4-b]-1,3,4-thiadiazines I [R1 = 4-Cl, 2,4-Cl2, 3,4-(OCH2O), 3,4-(MeO)2; X = O, NH; R2 = H, 2-Cl, 4-Cl-3-Me, 2,4-Cl2, 3-Cl-4-F; R3 = 2,4-Cl2-5-FC6H2] was synthesized by the condensation of 1,3-diaryl-2-bromo-1-propenones II with the corresponding 3-substituted 4-amino-5-mercapto-1,2,4-triazoles III. These compds. were tested for their antimicrobial activities against Escherichia coli, Staphylococcus aureus (Smith), Pseudomonas aeruginosa (Gessard), Bacillus subtilis and Candida albicans. Some of the newly synthesized compds. were also screened for their anticancer activity. Among these compds., I [R1 = 3,4-(OCH2O); X = NH; R2 = 4-Cl] and I (R1 = 4-Cl; X = O; R2 = 2-Cl, 4-Cl-3-Me) showed in vitro anticancer activity.

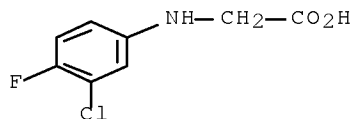
IT 83442-58-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of fluorine-containing (arylidene)triazolothiadiazines as antibacterial, antifungal and anticancer agents via heterocyclization of diaryl(bromo)propenones with amino(mercapto)triazoles)

RN 83442-58-4 ZCAPLUS

CN Glycine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 13 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:464826 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:488666

TITLE: Preparation of quinoline, tetrahydroquinazoline, and pyrimidine derivatives as MCH antagonist for treatment of CNS disorders

10/598508

INVENTOR(S): Sekiguchi, Yoshinori; Kanuma, Yukihiro; Omodera, Katsunori; Busujima, Takeshi; Tran, Thuy-Ahn; Han, Sangdong; Casper, Martin; Brian, A. Kramer; Semple, Graeme; Zou, Ning

PATENT ASSIGNEE(S): Taisho Pharmaceutical Co., Ltd., Japan; Arena Pharmaceutical Inc.

SOURCE: Jpn. Kokai Tokkyo Koho, 781 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

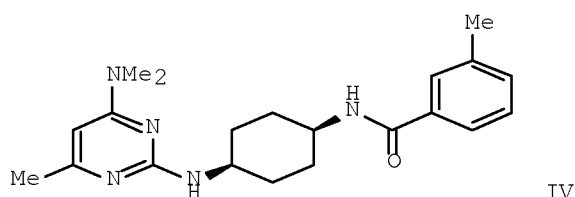
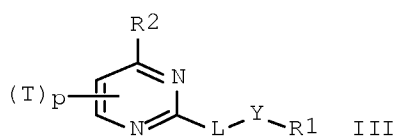
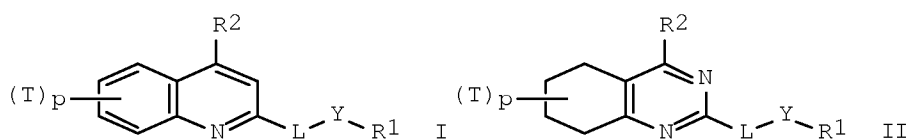
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006124387	A	20060518	JP 2005-286311	20050930
PRIORITY APPLN. INFO.:			JP 2004-287659	A 20040930
OTHER SOURCE(S):	MARPAT 144:488666			

GI



AB Title compds. [I, II, III; wherein R1 = (un)substituted (cyclo)alkyl, (cyclo)alkenyl, alkynyl, aryl; R2 = H, halo, OH, carboxy, carbamoyl, amino, (un)substituted alkyl, alkoxy; T = independently H, halo, OH, carboxy, carbamoyl, amino, cyano, NO2, alkenyl, alkynyl, cycloalkyl, (un)substituted alkyl, alkoxy; p = 0-5; L = aminocycloalkylideneamino, etc.; Y = bond, CH2, CO2, OCO, SO2, CO, CS, CONH, CSNH, etc.; with provisos; and pharmaceutically acceptable salts, hydrates, or solvates thereof] were prepared as antagonists of melanin concentrating hormone (MCH), an endogenous ligand of G-protein coupled receptors (GPCRs). Examples include solution and solid phase general synthetic methods and phys. data for nearly 3400 invention compds. In addition, all exemplified compds. were assayed using high throughput functional screening to detect intracellular Ca2+ concns. for accessing GPCR activation. For instance, reaction of 2,4-dichloro-6-methylpyrimidine with dimethylamine gave 2-chloro-4-(dimethylamino)-6-methylpyrimidine (40%), which

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was coupled with cis-(4-aminocyclohexyl)carbamic acid tert-Bu ester (60%). Deprotection (72%), amidation, and workup provided the benzamide (IV)•TFA. The latter demonstrated MCH antagonist activity with an IC50 value of 7.6 nM. Thus, pharmaceutical compns. comprising I are useful for the prophylaxis or treatment of improving memory function, sleeping and arousal, anxiety, depression, mood disorders, seizure, obesity, diabetes, appetite and eating disorders, cardiovascular disease, hypertension, dyslipidemia, myocardial infarction, binge eating disorders including bulimia, anorexia, mental disorders including manic depression, schizophrenia, delirium, dementia, stress, cognitive disorders, attention deficit disorder, substance abuse disorders, and dyskinesias including Parkinson's disease, epilepsy, and addiction (no data).

IT 771545-68-7P 773142-36-2P 773142-42-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(MCH antagonist; preparation of quinolines, quinazolines, and pyrimidines

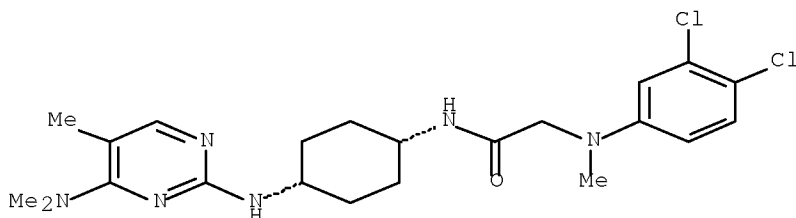
as

MCH antagonist for treatment of CNS disorders)

RN 771545-68-7 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)methylamino]-N-[cis-4-[[4-(dimethylamino)-5-methyl-2-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

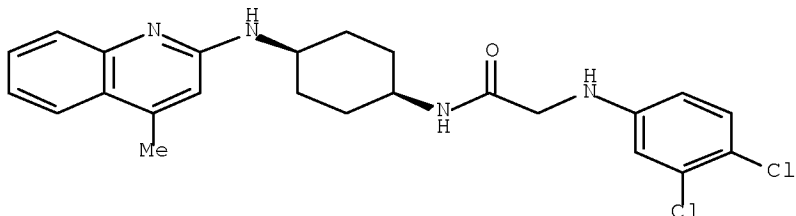
Relative stereochemistry.



RN 773142-36-2 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-[cis-4-[(4-methyl-2-quinolinyl)amino]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

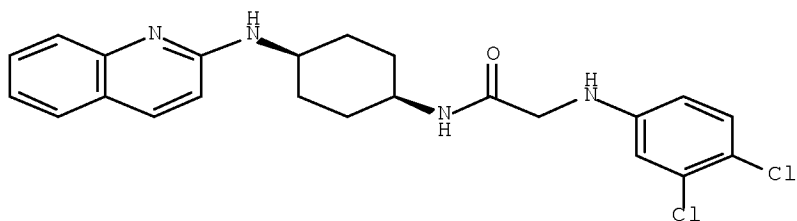


RN 773142-42-0 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-[cis-4-(2-quinolinylamino)cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

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IT 771545-69-8P 771551-46-3P 771554-02-0P
771554-83-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(melanin-concentrating hormone antagonist; preparation of quinolines,
quinazolines,
and pyrimidines as melanin-concentrating hormone antagonist for treatment
of
CNS disorders)

RN 771545-69-8 ZCAPLUS

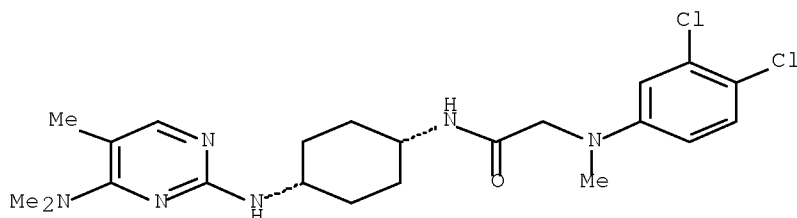
CN Acetamide, 2-[(3,4-dichlorophenyl)methylamino]-N-[cis-4-[[4-
(dimethylamino)-5-methyl-2-pyrimidinyl]amino]cyclohexyl]-,
2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 771545-68-7

CMF C22 H30 Cl2 N6 O

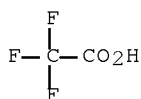
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2

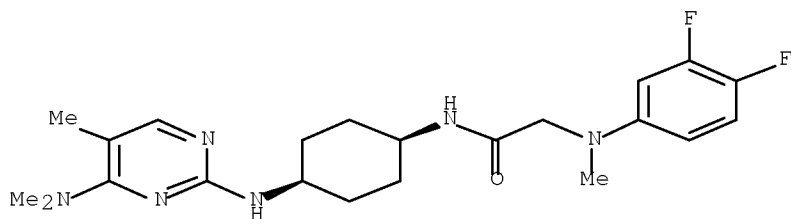


10/598508

RN 771551-46-3 ZCAPLUS

CN Acetamide, 2-[(3,4-difluorophenyl)methylamino]-N-[cis-4-[[4-(dimethylamino)-5-methyl-2-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

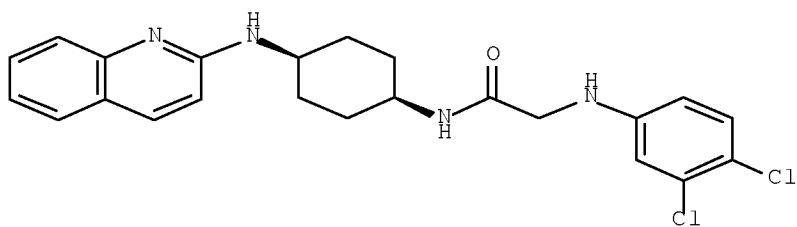
Relative stereochemistry.



RN 771554-02-0 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-[cis-4-(2-quinolinylamino)cyclohexyl]-, hydrochloride (1:2) (CA INDEX NAME)

Relative stereochemistry.

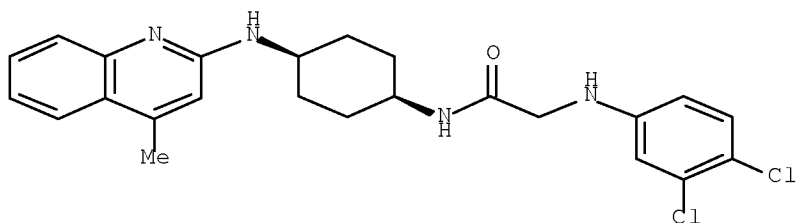


●2 HCl

RN 771554-83-7 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-[cis-4-[(4-methyl-2-quinolinyl)amino]cyclohexyl]-, hydrochloride (1:2) (CA INDEX NAME)

Relative stereochemistry.



●2 HCl

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L58 ANSWER 14 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:383697 ZCAPLUS Full-text

DOCUMENT NUMBER: 144:432552

TITLE: Preparation of substituted anilines as selective androgen receptor modulators

INVENTOR(S): Turnbull, Philip Stewart; Larkin, Andrew Lamont; Kaldor, Istvan; Cadilla, Rodolfo; Cowan, David John; Stewart, Eugene Lee

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 134 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

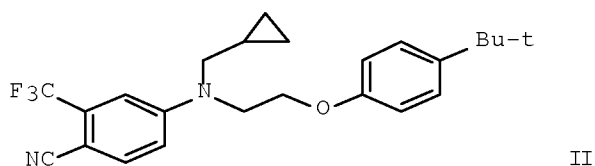
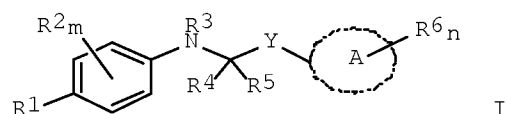
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006044707	A1	20060427	WO 2005-US37094	20051013
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
EP 1809275	A1	20070725	EP 2005-812180	20051013
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR			
JP 2008515998	T	20080515	JP 2007-536962	20051013
PRIORITY APPLN. INFO.:			US 2004-618480P	P 20041013
			WO 2005-US37094	W 20051013
OTHER SOURCE(S):		CASREACT 144:432552; MARPAT 144:432552		

GI

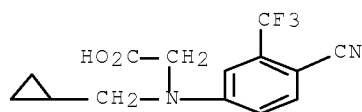


AB This invention relates to non-steroidal compds. I [R1 = CN or NO2; R2 = independently CN, NO2, halo, etc.; R3 = H, (cyclo)alkyl, alkoxy-carbonylalkyl, etc.; R4, R5 = independently H, (cyclo)alkyl, halo, etc., or R4R5 = (un)substituted (hetero)cyclyl; Y = (un)substituted methylene(oxy), methylenethio, carbonylamino, etc.; A = (hetero)aryl or heterocyclyl; m = 0-2; n = 0-5; R6 = independently (halo)alkyl, halo, hydroxy, etc.] which are or are believed to be modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, and also to the methods for the making and use of such compds. For example, II was provided in a multi-step synthesis starting from the reaction of 4-fluoro-2-(trifluoromethyl)benzonitrile with 1-cyclopropylmethanamine. The compds. I are claimed to be useful in the treatment or prophylaxis of conditions or disorders that respond to selective androgen receptor modulation (no data given).

IT 864283-36-3P, N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)glycine 864283-41-0P, N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-ethylglycine 864283-47-6P, N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)glycine 864283-49-8P, Methyl N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)glycinate 864283-71-6P, 2-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]butanoic acid 864283-86-3P, N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-propylglycine 864283-96-5P, 1,1-Dimethylethyl N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2-propen-1-yl)glycinate 864284-07-1P, N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-isobutylglycine 864284-25-3P, N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)alanine
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of substituted aniline derivs. as selective androgen receptor modulators)

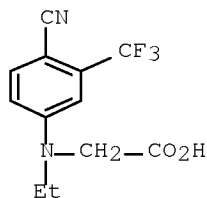
RN 864283-36-3 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)- (CA INDEX NAME)



RN 864283-41-0 ZCAPLUS

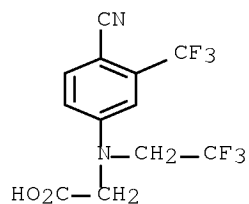
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-ethyl- (CA INDEX NAME)



RN 864283-47-6 ZCAPLUS

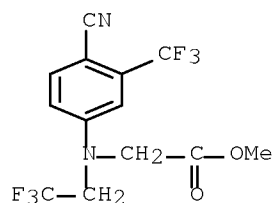
10/598508

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-
(CA INDEX NAME)



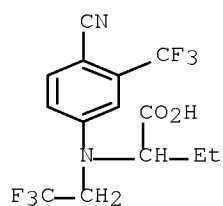
RN 864283-49-8 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-,
methyl ester (CA INDEX NAME)



RN 864283-71-6 ZCAPLUS

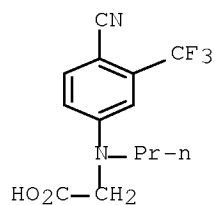
CN Butanoic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



RN 864283-86-3 ZCAPLUS

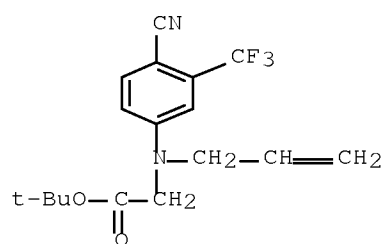
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-propyl- (CA INDEX NAME)

10/598508



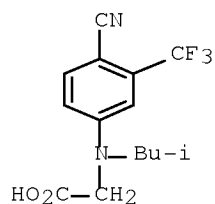
RN 864283-96-5 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-2-propen-1-yl-,
1,1-dimethylethyl ester (CA INDEX NAME)



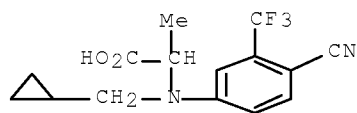
RN 864284-07-1 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2-methylpropyl)- (CA
INDEX NAME)



RN 864284-25-3 ZCAPLUS

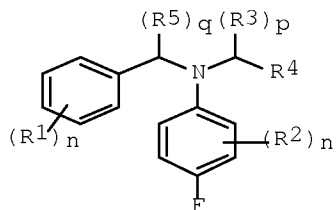
CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)- (CA
INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

L58 ANSWER 15 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:1075546 ZCAPLUS Full-text
 DOCUMENT NUMBER: 143:346900
 TITLE: Preparation of aniline derivatives as mitotic kinesin inhibitors
 INVENTOR(S): Garbaccio, Robert M.; Olson, Christy M.; Tasber, Edward S.; Torrent, Maricel
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: PCT Int. Appl., 54 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005092011	A2	20051006	WO 2005-US9198	20050318
WO 2005092011	A3	20051124		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2005226670	A1	20051006	AU 2005-226670	20050318
CA 2560213	A1	20051006	CA 2005-2560213	20050318
EP 1730099	A2	20061213	EP 2005-754102	20050318
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, LV			
CN 1934066	A	20070321	CN 2005-80009351	20050318
JP 2007530545	T	20071101	JP 2007-505031	20050318
IN 2006DN05527	A	20070824	IN 2006-DN5527	20060922
PRIORITY APPLN. INFO.:			US 2004-555164P	P 20040322
			WO 2005-US9198	W 20050318
OTHER SOURCE(S):	MARPAT 143:346900			
GI				



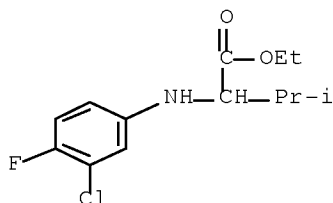
I

AB Title compds. I [n = 0-4; p = 1-2; q = 0-1; R1 = H, halo, alkyl, OH, etc.; R2 = H, halo; R3-4 = H, CF3, oxo, OH, halo, etc.; R5 = H, alkyl] are prepared For instance, 3-[[[(3-chloro-4-fluorophenyl)(2-hydroxy-1-methylethyl)amino]methyl]phenol is prepared in 3 steps from Me pyruvate, 3-chloro-4-fluoroaniline and 3-hydroxybenzaldehyde. In a kinesin ATPase in-vitro assay, compds. of the invention have an IC50 ≤ 30 μM. I are useful in the treatment of cancer.

IT 866030-16-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of aniline derivs. as mitotic kinesin inhibitors)

RN 866030-16-2 ZCAPLUS

CN Valine, N-(3-chloro-4-fluorophenyl)-, ethyl ester (CA INDEX NAME)



L58 ANSWER 16 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1004698 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:286689

TITLE: Preparation of aniline amino acid derivatives as selective androgen receptor modulators

INVENTOR(S): Turnbull, Phillip Stewart; Cadilla, Rodolfo; Cowan, David John; Larkin, Andrew Lamont; Kaldor, Istvan; Stewart, Eugene Lee

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 120 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085185	A1	20050915	WO 2005-US7245	20050303
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1725522	A1	20061129	EP 2005-730067	20050303

10/598508

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV

JP 2007526336 T 20070913 JP 2007-502061 20050303

US 20070191479 A1 20070816 US 2006-598508 20060901

PRIORITY APPLN. INFO.: US 2004-549794P P 20040303

WO 2005-US7245 W 20050303

OTHER SOURCE(S): CASREACT 143:286689; MARPAT 143:286689

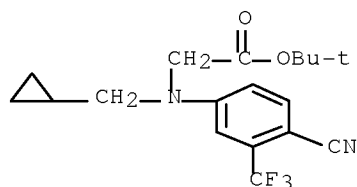
AB The invention relates to non-steroidal compds. 3,4-R4R3C6H3NR1R2 [R1 is - (Q1)0-1-R5, where Q1 is alkylene and R5 is H, alkyl, alkenyl, alkynyl, haloalkyl or cycloalkyl; R2 is -Q3-Q4-R6 or -Q3-CN, where Q3 is alkylene, Q4 is CO, CS, C:NR7, R7 is H or alkyl; R6 is alkyl, alkenyl, alkynyl, hydroxy, alkoxy, aryloxy or an amino group; R3 is CN, NO2 or halo; R4 is CN, NO2, halo, haloalkyl, alkyl, alkenyl, alkynyl, hydroxy, alkoxy, aryl or aryloxy] and their salts, solvates and physiol. functional derivs., that are modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, as well as methods for their synthesis and use. Thus, N2-[4-cyano-3-(trifluoromethyl)phenyl]-N2-(cyclopropylmethyl)-N1-methylglycinamide was prepared from 4-fluoro-2-(trifluoromethyl)benzonitrile by reaction with cyclopropylmethylamine and tert-Bu bromoacetate, followed by ester cleavage and methylamidation.

IT 864283-35-2P 864283-36-3P 864283-40-9P
864283-41-0P 864283-46-5P 864283-47-6P
864283-48-7P 864283-57-8P 864283-58-9P
864283-59-0P 864283-68-1P 864283-71-6P
864283-84-1P 864283-86-3P 864283-99-8P
864284-04-8P 864284-22-0P 864284-40-2P
864284-44-6P 864284-52-6P 864284-55-9P
864284-74-2P 864284-76-4P 864284-84-4P
864284-95-7P 864285-03-0P 864285-13-2P
864285-15-4P 864285-17-6P 864285-25-6P
864285-37-0P 864285-45-0P 864285-47-2P
864285-55-2P 864285-57-4P 864285-65-4P
864285-67-6P 864285-69-8P 864285-77-8P
864285-79-0P 864285-85-8P 864285-87-0P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of aniline amino acid derivs. as selective androgen receptor modulators)

RN 864283-35-2 ZCAPLUS

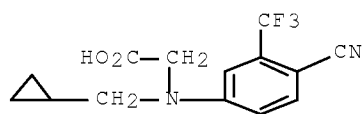
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864283-36-3 ZCAPLUS

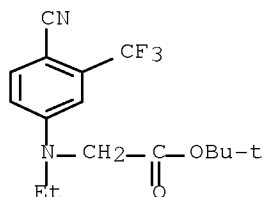
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)- (CA INDEX NAME)

10/598508



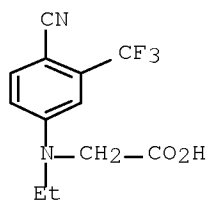
RN 864283-40-9 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-ethyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



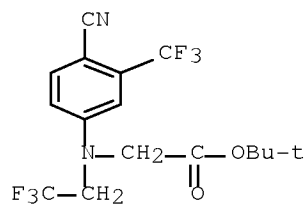
RN 864283-41-0 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-ethyl- (CA INDEX NAME)



RN 864283-46-5 ZCAPLUS

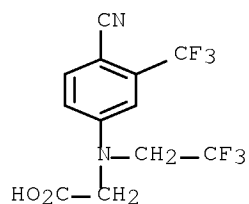
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864283-47-6 ZCAPLUS

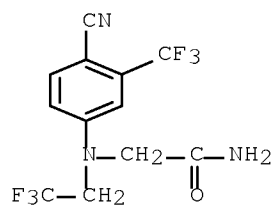
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

10/598508



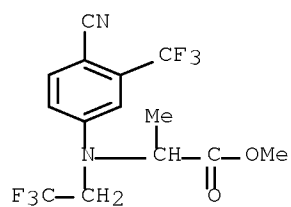
RN 864283-48-7 ZCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



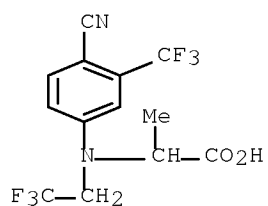
RN 864283-57-8 ZCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, methyl ester (CA INDEX NAME)



RN 864283-58-9 ZCAPLUS

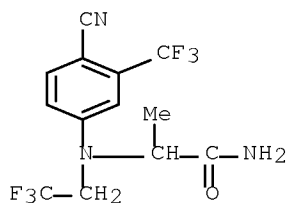
CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



10/598508

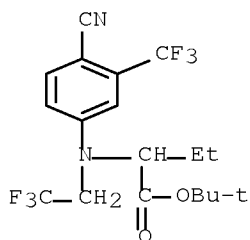
RN 864283-59-0 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



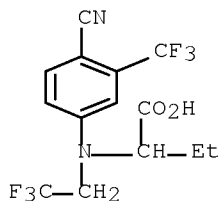
RN 864283-68-1 ZCAPLUS

CN Butanoic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864283-71-6 ZCAPLUS

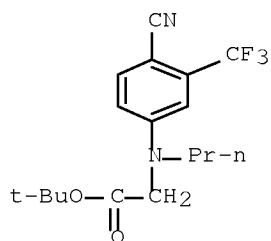
CN Butanoic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



RN 864283-84-1 ZCAPLUS

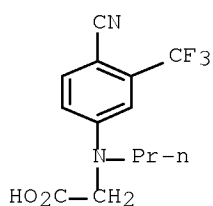
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-propyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

10/598508



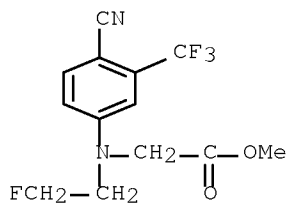
RN 864283-86-3 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-propyl- (CA INDEX NAME)



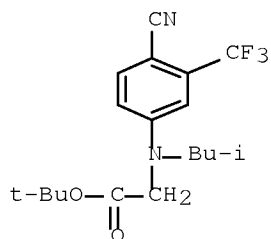
RN 864283-99-8 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2-fluoroethyl)-, methyl ester (CA INDEX NAME)



RN 864284-04-8 ZCAPLUS

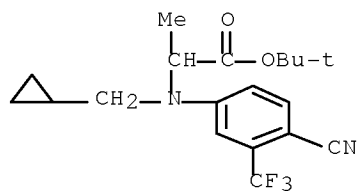
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2-methylpropyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



10/598508

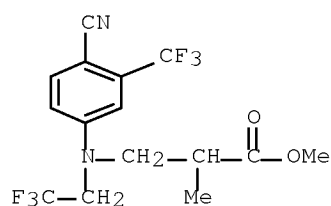
RN 864284-22-0 ZCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



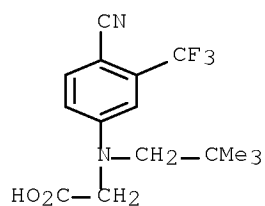
RN 864284-40-2 ZCAPLUS

CN Propanoic acid, 3-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-2-methyl-, methyl ester (CA INDEX NAME)



RN 864284-44-6 ZCAPLUS

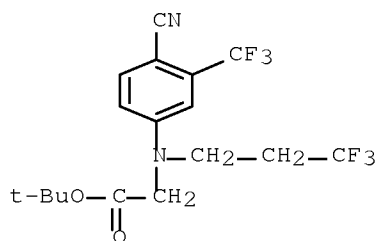
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2-dimethylpropyl)- (CA INDEX NAME)



RN 864284-52-6 ZCAPLUS

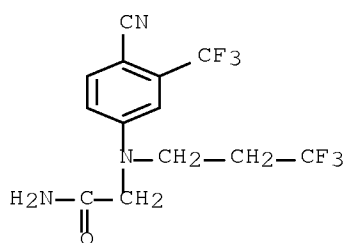
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(3,3,3-trifluoropropyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

10/598508



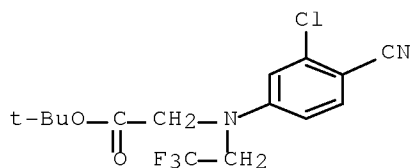
RN 864284-55-9 ZCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](3,3,3-trifluoropropyl)amino]- (CA INDEX NAME)



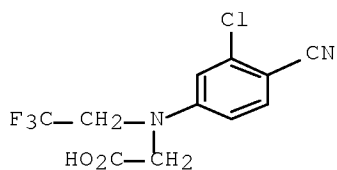
RN 864284-74-2 ZCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864284-76-4 ZCAPLUS

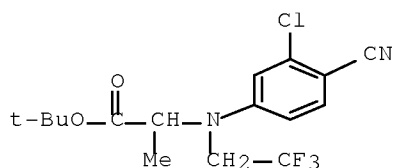
CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



10/598508

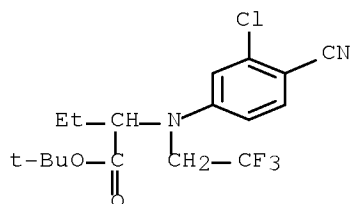
RN 864284-84-4 ZCAPLUS

CN Alanine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



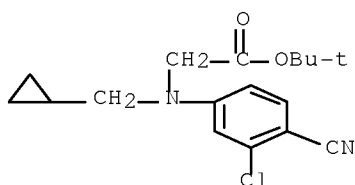
RN 864284-95-7 ZCAPLUS

CN Butanoic acid, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)



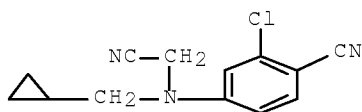
RN 864285-03-0 ZCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864285-13-2 ZCAPLUS

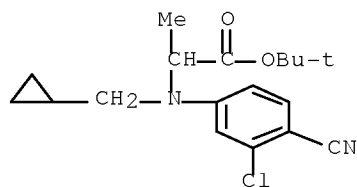
CN Benzonitrile, 2-chloro-4-[(cyanomethyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)



10/598508

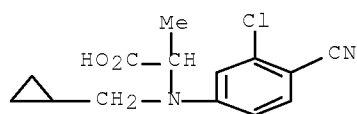
RN 864285-15-4 ZCAPLUS

CN Alanine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)-,
1,1-dimethylethyl ester (CA INDEX NAME)



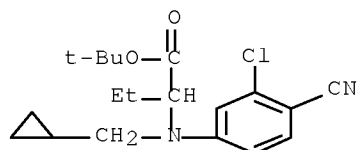
RN 864285-17-6 ZCAPLUS

CN Alanine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)- (CA INDEX
NAME)



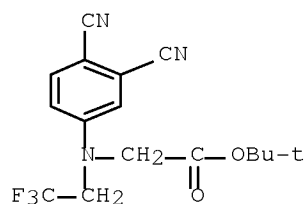
RN 864285-25-6 ZCAPLUS

CN Butanoic acid, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-,
1,1-dimethylethyl ester (CA INDEX NAME)



RN 864285-37-0 ZCAPLUS

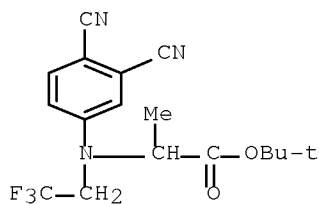
CN Glycine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)-,
1,1-dimethylethyl ester (CA INDEX NAME)



10/598508

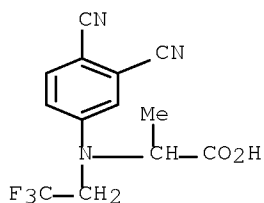
RN 864285-45-0 ZCAPLUS

CN Alanine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)-,
1,1-dimethylethyl ester (CA INDEX NAME)



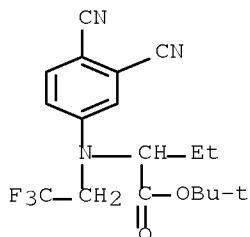
RN 864285-47-2 ZCAPLUS

CN Alanine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



RN 864285-55-2 ZCAPLUS

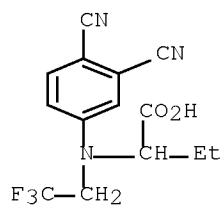
CN Butanoic acid, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-,
1,1-dimethylethyl ester (CA INDEX NAME)



RN 864285-57-4 ZCAPLUS

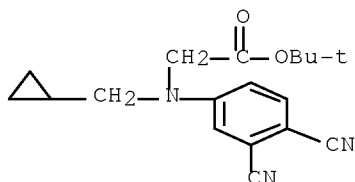
CN Butanoic acid, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA
INDEX NAME)

10/598508



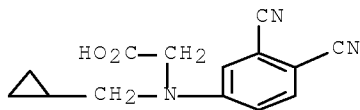
RN 864285-65-4 ZCAPLUS

CN Glycine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



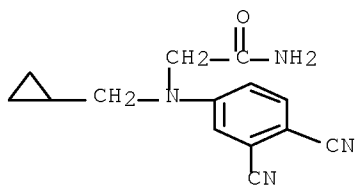
RN 864285-67-6 ZCAPLUS

CN Glycine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)- (CA INDEX NAME)



RN 864285-69-8 ZCAPLUS

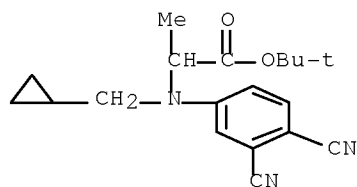
CN Acetamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]- (CA INDEX NAME)



RN 864285-77-8 ZCAPLUS

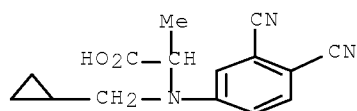
CN Alanine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

10/598508



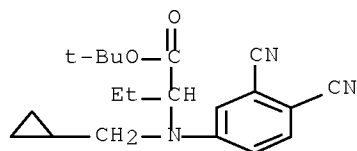
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CN Alanine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)- (CA INDEX NAME)



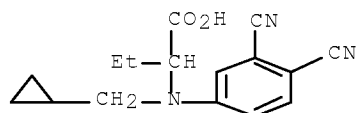
RN 864285-85-8 ZCAPLUS

CN Butanoic acid, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864285-87-0 ZCAPLUS

CN Butanoic acid, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]- (CA INDEX NAME)



IT 864283-37-4P 864283-38-5P 864283-39-6P
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 864283-45-4P 864283-49-8P 864283-50-1P
 864283-51-2P 864283-52-3P 864283-53-4P
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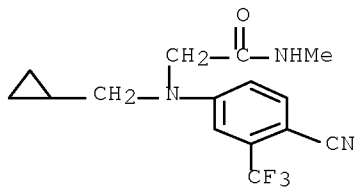
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of aniline amino acid derivs. as selective androgen receptor
modulators)

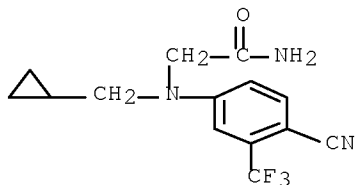
RN 864283-37-4 ZCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-
N-methyl- (CA INDEX NAME)



RN 864283-38-5 ZCAPLUS

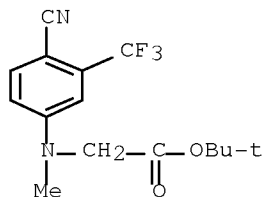
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-
(CA INDEX NAME)



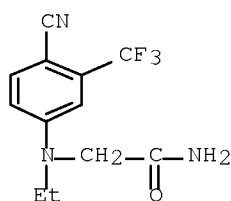
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CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-methyl-,
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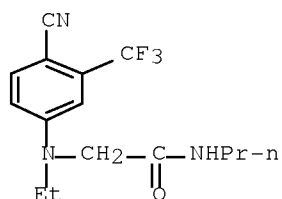
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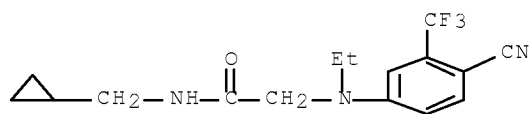
RN 864283-42-1 ZCAPLUS
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]ethylamino]- (CA INDEX NAME)



RN 864283-43-2 ZCAPLUS
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]ethylamino]-N-propyl- (CA INDEX NAME)



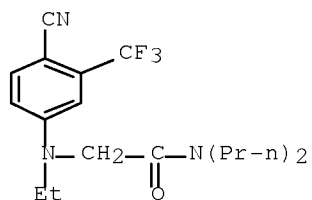
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CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]ethylamino]-N-(cyclopropylmethyl)- (CA INDEX NAME)



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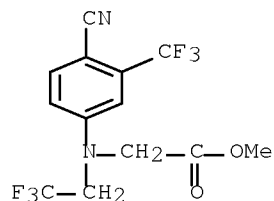
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CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]ethylamino]-N,N-dipropyl-
(CA INDEX NAME)



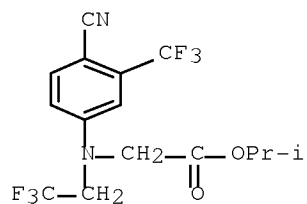
RN 864283-49-8 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-,
methyl ester (CA INDEX NAME)



RN 864283-50-1 ZCAPLUS

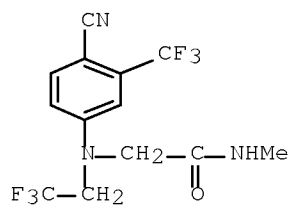
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-,
1-methylethyl ester (CA INDEX NAME)



RN 864283-51-2 ZCAPLUS

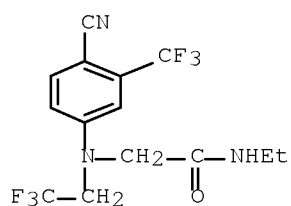
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-
trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

10/598508



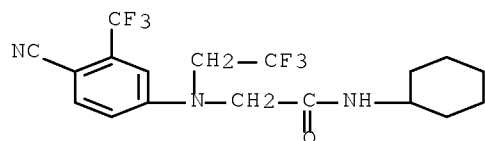
RN 864283-52-3 ZCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)



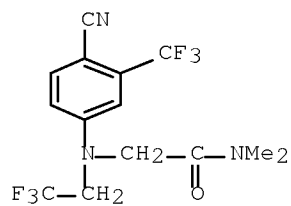
RN 864283-53-4 ZCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-cyclohexyl- (CA INDEX NAME)



RN 864283-54-5 ZCAPLUS

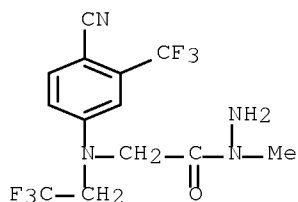
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)



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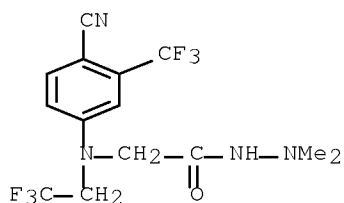
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CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-,
1-methylhydrazide (CA INDEX NAME)



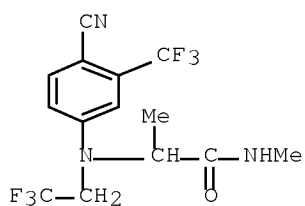
RN 864283-56-7 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-,
2,2-dimethylhydrazide (CA INDEX NAME)



RN 864283-60-3 ZCAPLUS

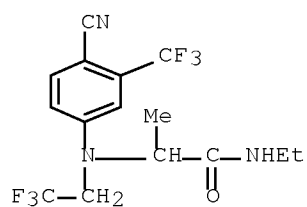
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)



RN 864283-62-5 ZCAPLUS

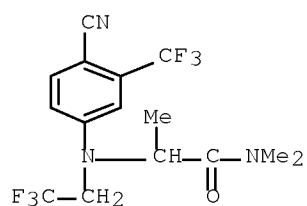
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)

10/598508



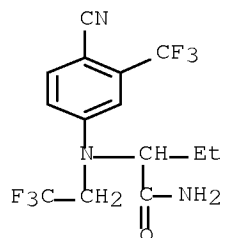
RN 864283-65-8 ZCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)



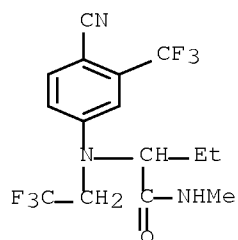
RN 864283-74-9 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



RN 864283-77-2 ZCAPLUS

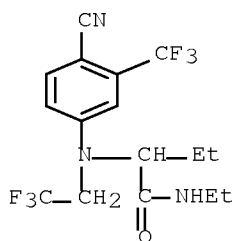
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)



10/598508

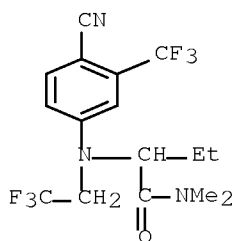
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CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)



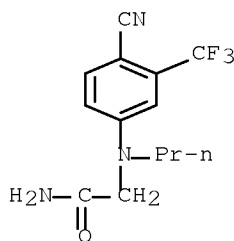
RN 864283-83-0 ZCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)



RN 864283-88-5 ZCAPLUS

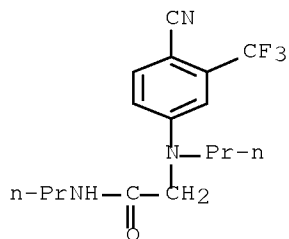
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]propylamino]- (CA INDEX NAME)



RN 864283-91-0 ZCAPLUS

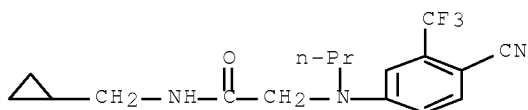
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]propylamino]-N-propyl- (CA INDEX NAME)

10/598508



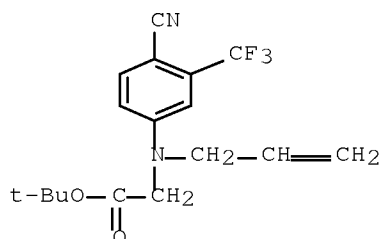
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CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]propylamino]-N-(cyclopropylmethyl)- (CA INDEX NAME)



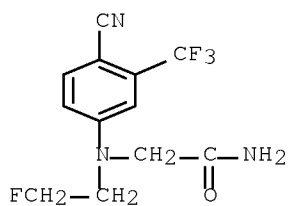
RN 864283-96-5 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-2-propen-1-yl-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864284-02-6 ZCAPLUS

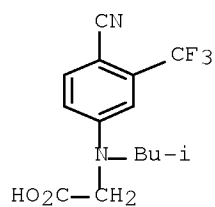
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2-fluoroethyl)amino]- (CA INDEX NAME)



10/598508

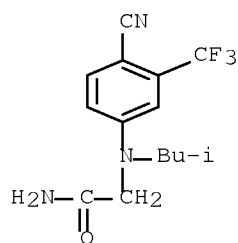
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CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2-methylpropyl)- (CA INDEX NAME)



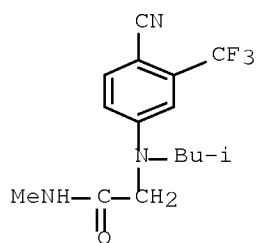
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CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2-methylpropyl)amino]- (CA INDEX NAME)



RN 864284-13-9 ZCAPLUS

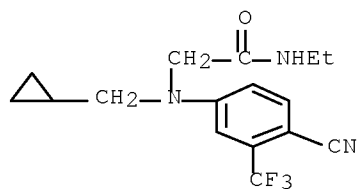
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2-methylpropyl)amino]-N-methyl- (CA INDEX NAME)



RN 864284-16-2 ZCAPLUS

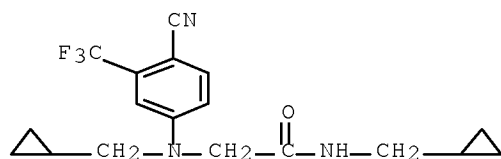
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-ethyl- (CA INDEX NAME)

10/598508



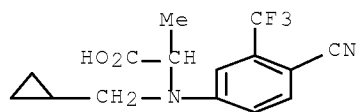
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CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]-(cyclopropylmethyl)amino]-N-(cyclopropylmethyl)- (CA INDEX NAME)



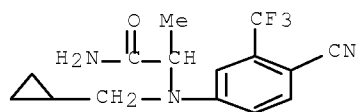
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CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)- (CA INDEX NAME)



RN 864284-27-5 ZCAPLUS

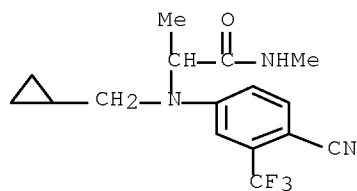
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]-(cyclopropylmethyl)amino]-N-methyl- (CA INDEX NAME)



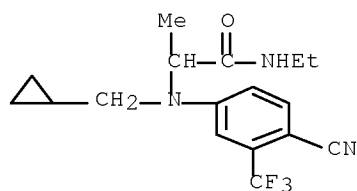
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CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]-(cyclopropylmethyl)amino]-N-methyl- (CA INDEX NAME)

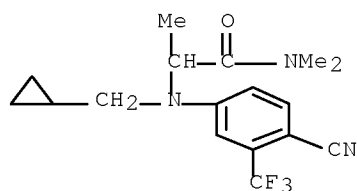
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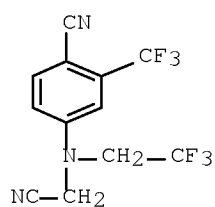
RN 864284-31-1 ZCAPLUS
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]-(cyclopropylmethyl)amino]-N-ethyl- (CA INDEX NAME)



RN 864284-33-3 ZCAPLUS
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl]-(cyclopropylmethyl)amino]-N,N-dimethyl- (CA INDEX NAME)



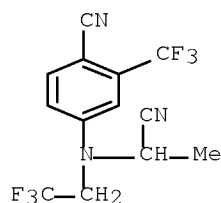
RN 864284-35-5 ZCAPLUS
CN Benzonitrile, 4-[(cyanomethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 864284-37-7 ZCAPLUS
CN Benzonitrile, 4-[(1-cyanoethyl)(2,2,2-trifluoroethyl)amino]-2-

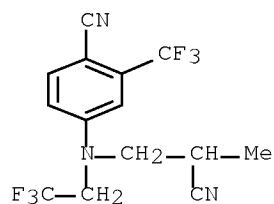
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(trifluoromethyl)- (CA INDEX NAME)



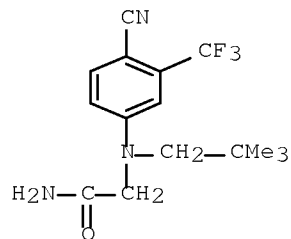
RN 864284-42-4 ZCAPLUS

CN Benzonitrile, 4-[(2-cyanopropyl) (2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 864284-46-8 ZCAPLUS

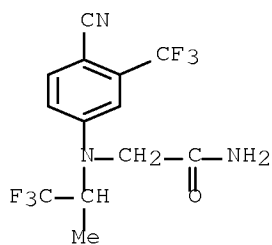
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl] (2,2-dimethylpropyl)amino]- (CA INDEX NAME)



RN 864284-48-0 ZCAPLUS

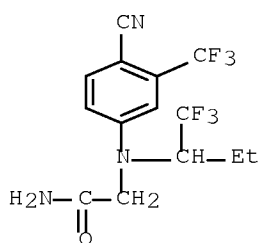
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl] (2,2,2-trifluoro-1-methylethyl)amino]- (CA INDEX NAME)

10/598508



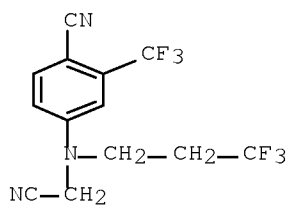
RN 864284-50-4 ZCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl][1-(trifluoromethyl)propyl]amino]- (CA INDEX NAME)



RN 864284-57-1 ZCAPLUS

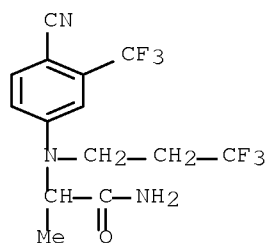
CN Benzonitrile, 4-[(cyanomethyl)(3,3,3-trifluoropropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 864284-59-3 ZCAPLUS

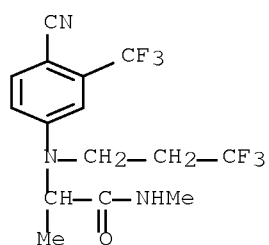
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](3,3,3-trifluoropropyl)amino]- (CA INDEX NAME)

10/598508



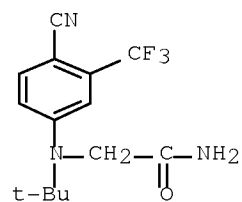
RN 864284-62-8 ZCAPLUS

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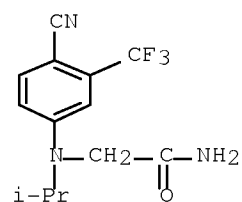
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CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](1,1-dimethylethyl)amino]- (CA INDEX NAME)



RN 864284-66-2 ZCAPLUS

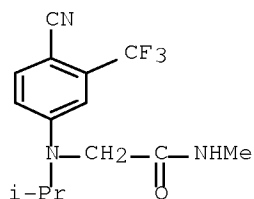
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](1-methylethyl)amino]- (CA INDEX NAME)



10/598508

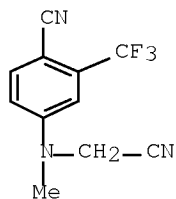
RN 864284-68-4 ZCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](1-methylethyl)amino]-N-methyl- (CA INDEX NAME)



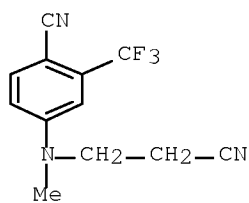
RN 864284-70-8 ZCAPLUS

CN Benzonitrile, 4-[(cyanomethyl)methylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 864284-72-0 ZCAPLUS

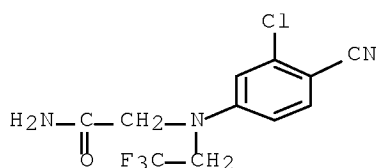
CN Benzonitrile, 4-[(2-cyanoethyl)methylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



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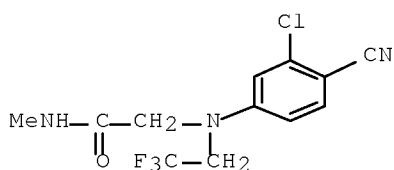
CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

10/598508



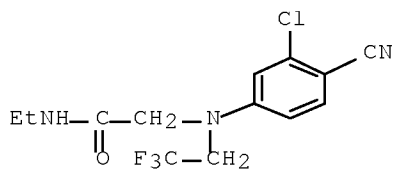
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CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)



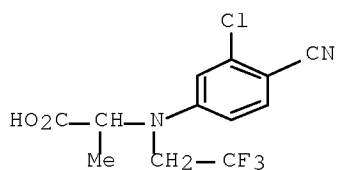
RN 864284-82-2 ZCAPLUS

CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)



RN 864284-87-7 ZCAPLUS

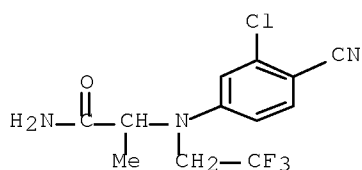
CN Alanine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



RN 864284-89-9 ZCAPLUS

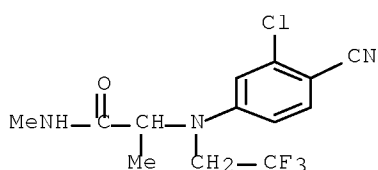
CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

10/598508



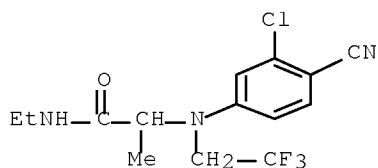
RN 864284-91-3 ZCAPLUS

CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)



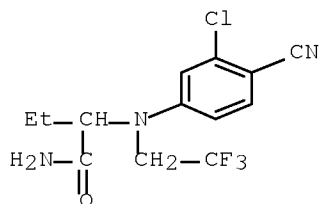
RN 864284-93-5 ZCAPLUS

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RN 864284-97-9 ZCAPLUS

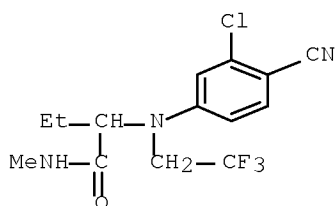
CN Butanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



10/598508

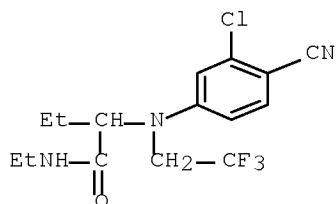
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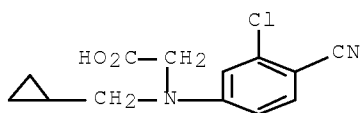
RN 864285-01-8 ZCAPLUS

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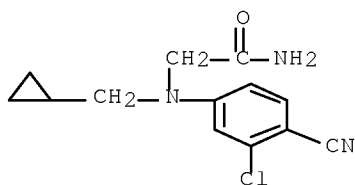
RN 864285-05-2 ZCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)- (CA INDEX NAME)



RN 864285-07-4 ZCAPLUS

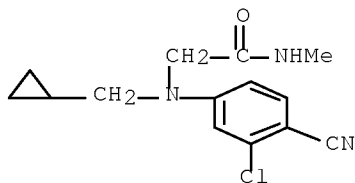
CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)



10/598508

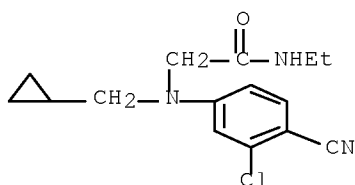
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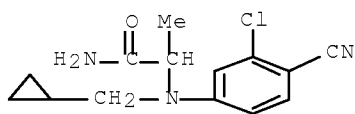
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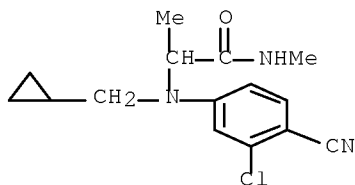
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CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]- (CA
INDEX NAME)



RN 864285-21-2 ZCAPLUS

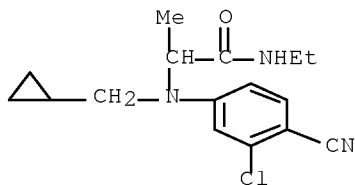
CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-N-methyl-
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10/598508

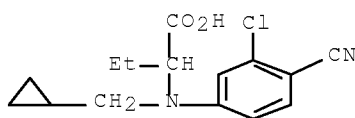
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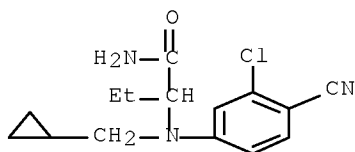
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CN Butanoic acid, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]- (CA
INDEX NAME)



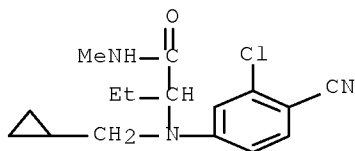
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INDEX NAME)



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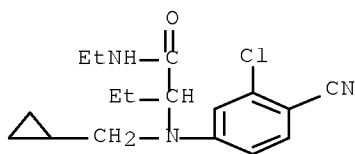
CN Butanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-N-methyl-
(CA INDEX NAME)



10/598508

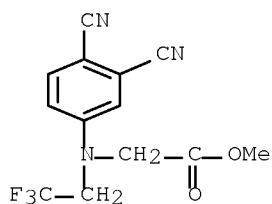
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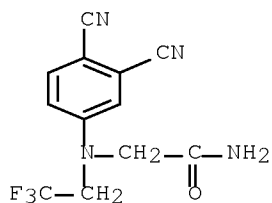
RN 864285-35-8 ZCAPLUS

CN Glycine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)-, methyl ester
(CA INDEX NAME)



RN 864285-39-2 ZCAPLUS

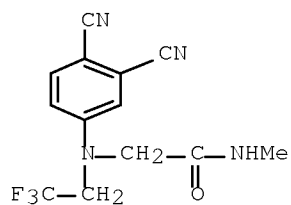
CN Acetamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX
NAME)



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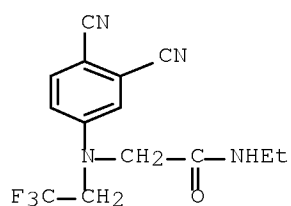
CN Acetamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl-
(CA INDEX NAME)

10/598508



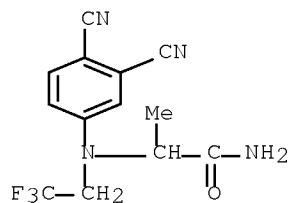
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CN Acetamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-ethyl-
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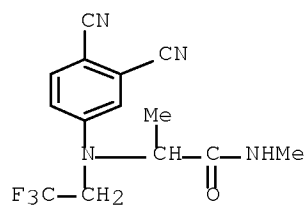
RN 864285-49-4 ZCAPLUS

CN Propanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-
(CA INDEX NAME)



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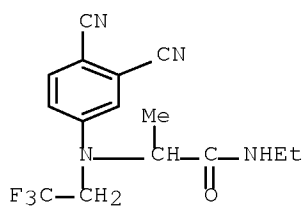
CN Propanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl-
(CA INDEX NAME)



10/598508

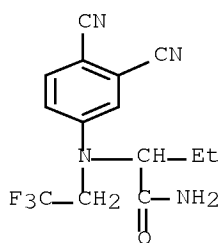
RN 864285-53-0 ZCAPLUS

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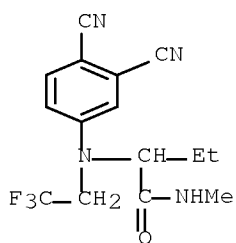
RN 864285-59-6 ZCAPLUS

CN Butanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX
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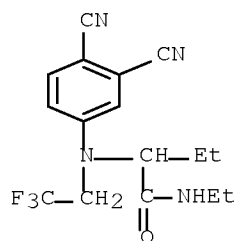
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RN 864285-63-2 ZCAPLUS

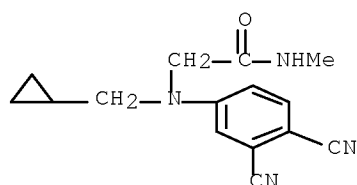
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(CA INDEX NAME)

10/598508



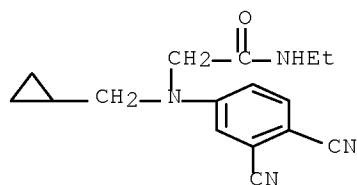
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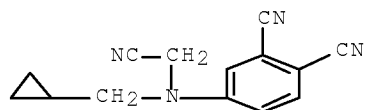
RN 864285-73-4 ZCAPLUS

CN Acetamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-ethyl- (CA INDEX NAME)



RN 864285-75-6 ZCAPLUS

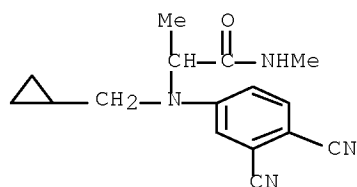
CN 1,2-Benzenedicarbonitrile, 4-[(cyanomethyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)



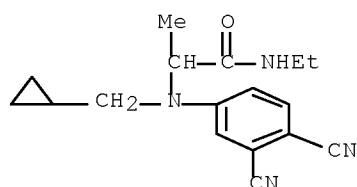
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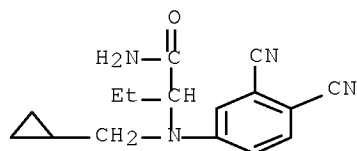
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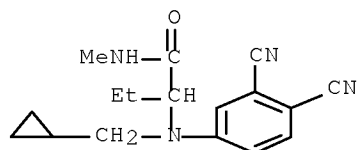
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CN Propanamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-ethyl- (CA INDEX NAME)



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CN Butanamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]- (CA INDEX NAME)

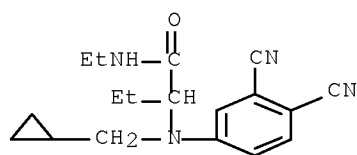


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CN Butanamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-methyl- (CA INDEX NAME)



RN 864285-93-8 ZCAPLUS
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10/598508



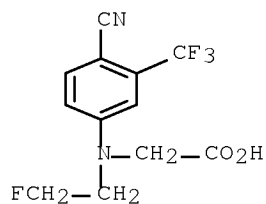
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864286-51-1P 864286-55-5P 864286-61-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of aniline amino acid derivs. as selective androgen receptor
modulators)

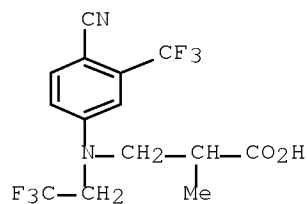
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CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2-fluoroethyl)- (CA
INDEX NAME)



RN 864286-10-2 ZCAPLUS

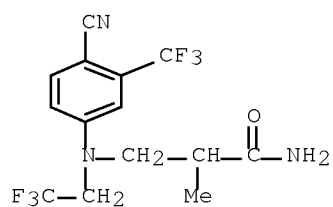
CN Propanoic acid, 3-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-
trifluoroethyl)amino]-2-methyl- (CA INDEX NAME)



RN 864286-12-4 ZCAPLUS

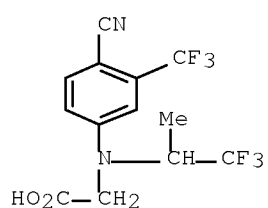
CN Propanamide, 3-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-
trifluoroethyl)amino]-2-methyl- (CA INDEX NAME)

10/598508



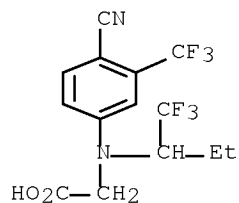
RN 864286-23-7 ZCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoro-1-methylethyl)- (CA INDEX NAME)



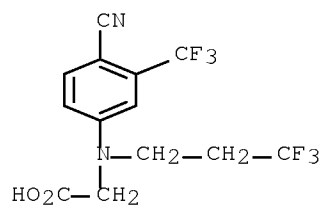
RN 864286-31-7 ZCAPLUS

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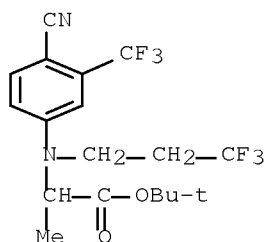
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



10/598508

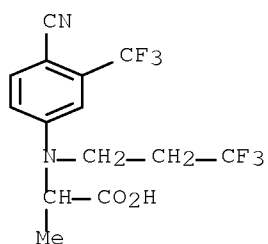
RN 864286-36-2 ZCAPLUS

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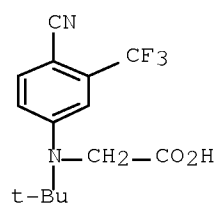
RN 864286-38-4 ZCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 864286-43-1 ZCAPLUS

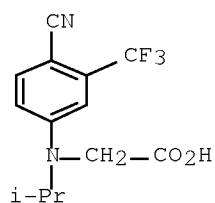
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(1,1-dimethylethyl)- (CA INDEX NAME)



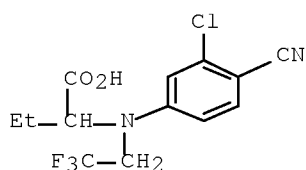
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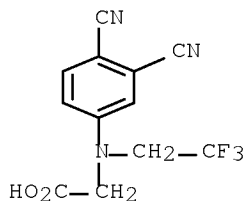
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RN 864286-55-5 ZCAPLUS
CN Butanoic acid, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-
(CA INDEX NAME)



RN 864286-61-3 ZCAPLUS
CN Glycine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 17 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:987987 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:267238
TITLE: Preparation of glycine ethyl ester-substituted
phthalonitrile
INVENTOR(S): Zhang, Fushi; Song, Zhenglin; Zhao, Fuqun; Niu, Lihong
PATENT ASSIGNEE(S): Tsinghua University, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 6 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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CN 1446798	A	20031008	CN 2002-116244	20020322
PRIORITY APPLN. INFO.:			CN 2002-116244	20020322
OTHER SOURCE(S):	CASREACT 143:267238			

AB The ethoxycarbonylmethylamino-substituted phthalonitrile is synthesized by substituting 4-amino-1,2-dibromobenzene with Et chloroacetate in alc. in the presence of NaOAc under bubbling N₂ and refluxing for 46-50 h and then substituting with CuCN in DMF at 140-160° for 7-9 h. The ethoxycarbonylmethylamino-substituted phthalonitrile may be used as the intermediate of glycine substituted phthalocyanine photosensitizing therapeutic agent.

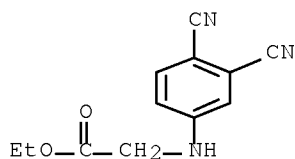
IT 863971-81-7P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of glycine Et ester-substituted phthalonitrile as intermediate for phthalocyanine photosensitizer)

RN 863971-81-7 ZCAPLUS

CN Glycine, N-(3,4-dicyanophenyl)-, ethyl ester (CA INDEX NAME)



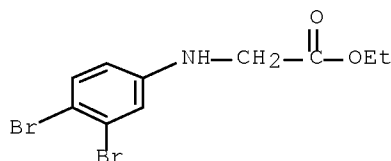
IT 863971-80-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of glycine Et ester-substituted phthalonitrile as intermediate for phthalocyanine photosensitizer)

RN 863971-80-6 ZCAPLUS

CN Glycine, N-(3,4-dibromophenyl)-, ethyl ester (CA INDEX NAME)



L58 ANSWER 18 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:431398 ZCAPLUS Full-text

DOCUMENT NUMBER: 142:463595

TITLE: Preparation of N-aminoalkyl amides as agonists of the κ opioid receptor useful against gastrointestinal disorders, pain, and pruritus

INVENTOR(S): Dolle, Roland E.; Chu, Guo-Hua; Gu, Minghua

PATENT ASSIGNEE(S): Adolor Corporation, USA

SOURCE: U.S. Pat. Appl. Publ., 46 pp.

CODEN: USXXCO

10/598508

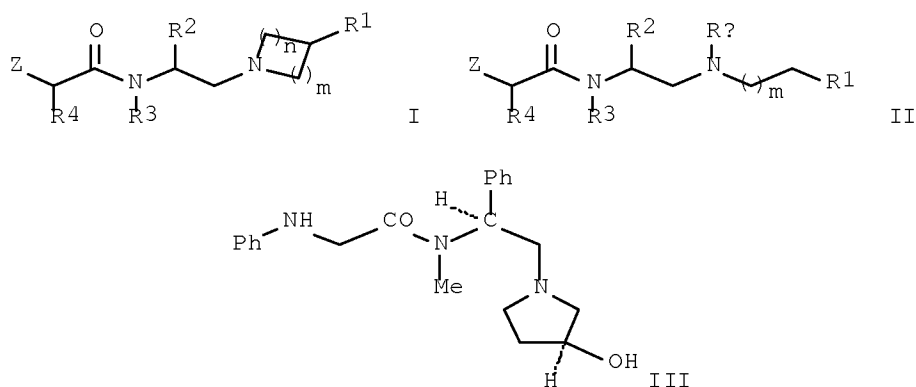
DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050107355	A1	20050519	US 2003-713746	20031114
US 7160902	B2	20070109		
WO 2005049564	A1	20050602	WO 2004-US37955	20041112

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

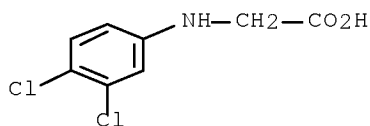
PRIORITY APPLN. INFO.: US 2003-713746 A 20031114
 OTHER SOURCE(S): CASREACT 142:463595; MARPAT 142:463595
 GI



AB Amide derivs. (shown as I and II; variables defined below; e.g. N-[2-((S)-3-hydroxypyrrolidin-1-yl)-(S)-1-phenylethyl]-N-methyl-2-phenylaminoacetamide (shown as III)) are disclosed. Pharmaceutical compns. containing these compds., and methods for their use, inter alia, for treating and/or preventing gastrointestinal disorders, pain, and pruritus (no data) are also disclosed. Although the methods of preparation are not claimed, 36 example preps. are included. For example, III was prepared (45 %) by coupling of N-phenylglycine with N-[2-((S)-3-hydroxypyrrolidin-1-yl)-(S)-1-phenylethyl]-N-methylamine dihydrochloride. For I and II: R1 is H or OH; R2 is alkyl, aryl, or aralkyl; R3 is alkyl, or R2 and R3 taken together with the atoms through which they are connected form a 4- to 8-membered heterocyclic ring; R4 is H, alkyl, cycloalkyl, alkylcycloalkyl, aryl, aralkyl, heteroaryl, or heteroarylalkyl; Z is -(CH₂)_nNR₅R₆ or -(CH₂)_nO-C(=O)-NR₇R₈; R₅ is H, alkyl, or

aryl; R6 is aryl, alkaryl, -CO(NH)pR9, or -SO2R9, provided that at least one of R5 and R6 is other than aryl; R7 is H or alkyl; R8 is alkyl, aryl, aralkyl, alkaryl, heteroaryl, heteroarylalkyl, cycloalkyl or cycloalkylalkyl; R9 is alkyl, cycloalkyl, alkylcycloalkyl, aryl, aralkyl, heteroaryl, or heteroarylalkyl; m is the integer 1, 2, or 3; n is the integer 1, 2, or 3; o is the integer 0, 1, 2, or 3; p is the integer 0 or 1; and the quantity (m+n) is an integer 2-5. Compds. in all the examples showed κ receptor affinity (K_i) $<10 \mu\text{M}$. For example, III had a $K_i = 0.17 \text{ nM}$ against the human κ receptor with $>100\times$ selectivity vs. the human μ and δ receptors and was an agonist with an $\text{EC}_{50} = 0.05 \text{ nM}$. It exhibited a % A = 96.2% at a dose of $300 \mu\text{g}$, i.paw in the in vivo formalin-induced nociception assay. This compound also blocked the action of HOAc-induced writhing when administered s.c. with an $\text{ED}_{50} = 0.017 \text{ mg/kg}$.

IT 851680-18-7P, (3,4-Dichlorophenylamino)acetic acid hydrochloride
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of N-aminoalkyl amides as agonists of κ opioid receptor useful against gastrointestinal disorders, pain, and pruritus)
 RN 851680-18-7 ZCAPLUS
 CN Glycine, N-(3,4-dichlorophenyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 19 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:99305 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 142:177127
 TITLE: Preparation of acylated amino acid amidyl pyrazoles and related compounds
 INVENTOR(S): Tung, Jay S.; Garofalo, Albert; Pleiss, Mike A.
 PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; Dressen, Darren; Guinn, Ashley C.; Jenkins, Scott A.; Latimer, Lee H.; Sealy, Jennifer
 SOURCE: PCT Int. Appl., 96 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005009344	A2	20050203	WO 2004-US18202	20040604
WO 2005009344	A3	20051006		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG

AU 2004258841 A1 20050203 AU 2004-258841 20040604

CA 2528496 A1 20050203 CA 2004-2528496 20040604

EP 1633350 A2 20060315 EP 2004-776373 20040604

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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JP 2006526621 T 20061124 JP 2006-509087 20040604

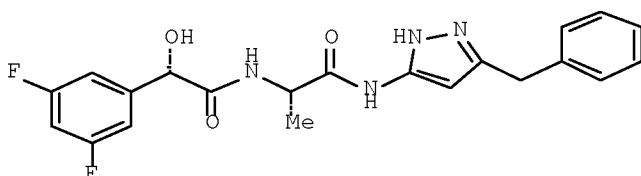
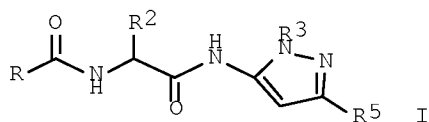
US 20070197624 A1 20070823 US 2007-559823 20070301

PRIORITY APPLN. INFO.: US 2003-476369P P 20030605

WO 2004-US18202 W 20040604

OTHER SOURCE(S): CASREACT 142:177127; MARPAT 142:177127

GI



II

AB The invention relates to acylated amino acid amidyl pyrazoles and related compds. I [R is (un)substituted aryl, cycloalkyl, heterocyclyl, alkoxy, cycloalkoxy, aryloxy, heteroaryloxy, alkylamino, cycloalkylamino, arylamino, heteroaryl amino or R1-Z-CX'X''-, where X', X'' are independently H, OH or F (provided that when one of X' and X'' is F, the other is not OH) or X'X'' is an oxo group, Z is alkyl, nitrogen, oxygen, sulfur or a bond and R1 is H, (un)substituted alkyl, alkenyl, aryl, cycloalkyl, cycloalkenyl, heteroaryl or heterocyclyl; R2 is H, alkyl, alkylalkoxy, alkylthioalkoxy, CO2H or an ester; R3 is H, (un)substituted alkyl, cycloalkyl or phenyl; R5 is -Y-R6, where Y is (un)substituted alkyl, alkenyl, aryl, cycloalkyl, cycloalkenyl, heteroaryl, heterocyclic or a bond and R6 is (un)substituted aryl, heteroaryl, cycloalkyl, heterocycloalkyl, aryl oxide, heteroaryl N-oxide or aryl sulfide (provided that when Y is a bond, then R6 is cycloalkyl or R2 is alkylalkoxy or alkylthioalkoxy)] or their pharmaceutically-acceptable salts, which are useful in the prevention and treatment of Alzheimer's disease. The invention is further directed to a method for inhibiting β -amyloid peptide release and/or synthesis, for inhibiting γ -secretase activity, and for treating neurol. disorders associated with β -amyloid peptide production. Thus, compound II was prepared by a multistep procedure starting from Boc-protected 4-

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phenyl-4-piperidinecarboxylic acid. The pyrazole ring was formed by reaction of a 4-(cyanoacetyl)-4- piperidine derivative with tert-BuNHNH2.HCl.

IT 834911-54-5P

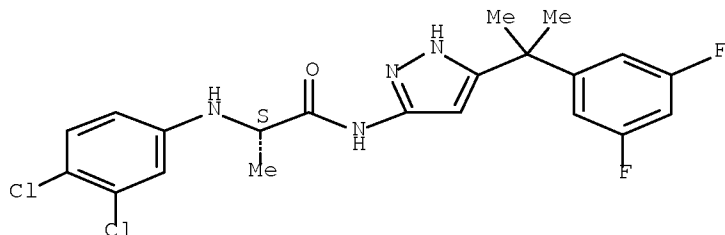
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acylated amino acid amidyl pyrazoles and related compds.)

RN 834911-54-5 ZCAPLUS

CN Propanamide, 2-[(3,4-dichlorophenyl)amino]-N-[5-[1-(3,5-difluorophenyl)-1-methylethyl]-1H-pyrazol-3-yl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 20 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:875033 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:332214

TITLE: Preparation of quinoline, tetrahydroquinazoline, and pyrimidine derivatives as MCH antagonist for treatment of CNS disorders

INVENTOR(S): Sekiguchi, Yoshinori; Kanuma, Kosuke; Omodera, Katsunori; Busujima, Tsuyoshi; Tran, Thuy-Anh; Han, Sangdon; Casper, Martin; Kramer, Bryan A.; Semple, Graeme; Zou, Ning

PATENT ASSIGNEE(S): Taisho Pharmaceutical Co. Ltd., Japan

SOURCE: Eur. Pat. Appl., 586 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

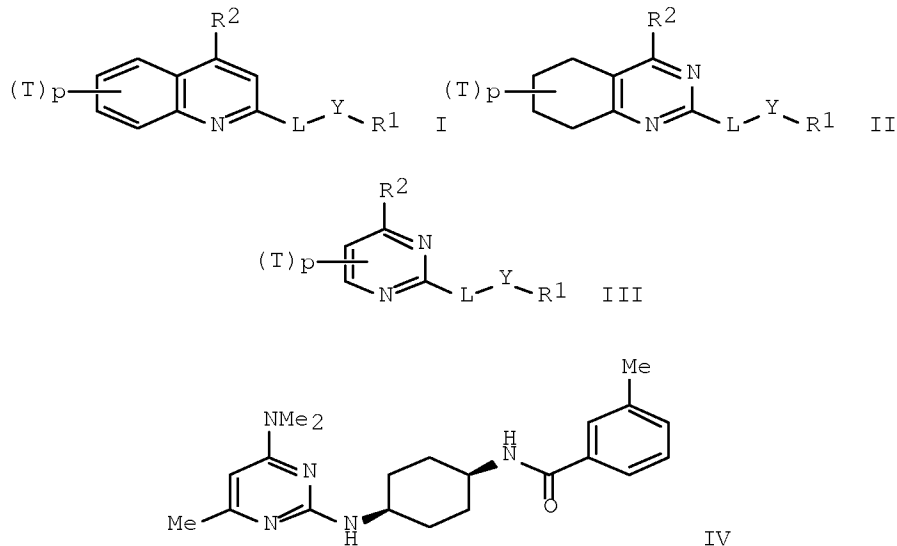
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1464335	A2	20041006	EP 2004-7651	20040330
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
EP 1464335	A2	20041006	EP 2004-7651	20040330
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
PRIORITY APPLN. INFO.:			US 2003-458530P	P 20030331
			US 2003-495911P	P 20030819
			US 2003-510186P	P 20031009
			US 2003-530360P	P 20031216
			EP 2004-7651	A 20040330

GI



AB Title compds. I, II, and III [wherein R1 = (un)substituted (cyclo)alkyl, (cyclo)alkenyl, alkynyl, aryl; R2 = H, halo, OH, carboxy, carbamoyl, amino, (un)substituted alkyl, alkoxy; T = independently H, halo, OH, carboxy, carbamoyl, amino, cyano, NO₂, alkenyl, alkynyl, cycloalkyl, (un)substituted alkyl, alkoxy; p = 0-5; L = aminocycloalkylideneamino, etc.; Y = bond, CH₂, CO₂, OCO, SO₂, CO, CS, CONH, CSNH, etc.; with provisos; and pharmaceutically acceptable salts, hydrates, or solvates thereof] were prepared as antagonists of melanin concentrating hormone (MCH), an endogenous ligand of G-protein coupled receptors (GPCRs). Examples include solution and solid phase general synthetic methods and phys. data for nearly 3400 invention compds. In addition, all exemplified compds. were assayed using high throughput functional screening to detect intracellular Ca²⁺ concns. for accessing GPCR activation. For instance, reaction of 2,4-dichloro-6-methylpyrimidine with dimethylamine gave 2-chloro-4-(dimethylamino)-6-methylpyrimidine (40%), which was coupled with cis-(4-aminocyclohexyl)carbamic acid tert-Bu ester (60%). Deprotection (72%), amidation, and workup provided the benzamide IV•TFA. The latter demonstrated MCH antagonist activity with an IC₅₀ value of 7.6 nM. Thus, pharmaceutical compns. comprising I are useful for the prophylaxis or treatment of improving memory function, sleeping and arousal, anxiety, depression, mood disorders, seizure, obesity, diabetes, appetite and eating disorders, cardiovascular disease, hypertension, dyslipidemia, myocardial infarction, binge eating disorders including bulimia, anorexia, mental disorders including manic depression, schizophrenia, delirium, dementia, stress, cognitive disorders, attention deficit disorder, substance abuse disorders, and dyskinesias including Parkinson's disease, epilepsy, and addiction (no data). This is part III of three in a series covering the patent.

IT 771545-68-7P 771551-46-3P 773142-36-2P,
2-(3,4-Dichlorophenylamino)-N-[cis-4-[(4-methylquinolin-2-yl)amino]cyclohexyl]acetamide 773142-42-0P, 2-(3,4-Dichlorophenylamino)-N-[cis-4-[(quinolin-2-yl)amino]cyclohexyl]acetamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

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(Uses)

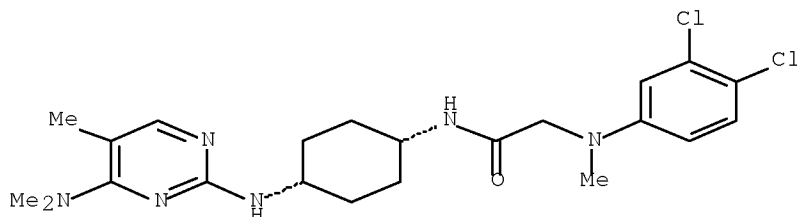
(MCH antagonist; preparation of quinolines, quinazolines, and pyrimidines
as

MCH antagonist for treatment of CNS disorders)

RN 771545-68-7 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)methylamino]-N-[cis-4-[[4-(dimethylamino)-5-methyl-2-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

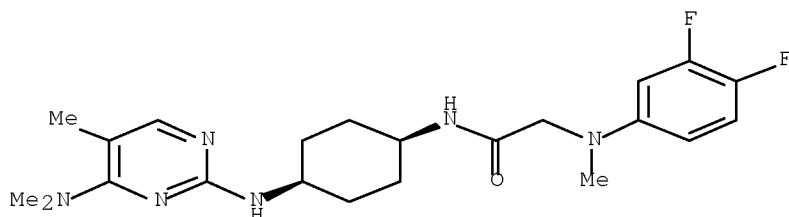
Relative stereochemistry.



RN 771551-46-3 ZCAPLUS

CN Acetamide, 2-[(3,4-difluorophenyl)methylamino]-N-[cis-4-[[4-(dimethylamino)-5-methyl-2-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

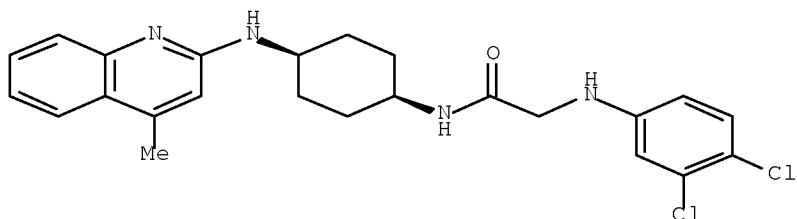
Relative stereochemistry.



RN 773142-36-2 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-[cis-4-[(4-methyl-2-quinolinyl)amino]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

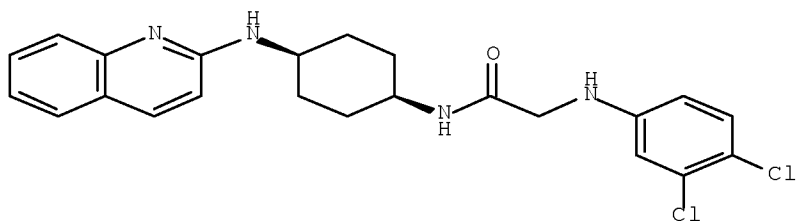


RN 773142-42-0 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-[cis-4-(2-quinolinylamino)cyclohexyl]- (CA INDEX NAME)

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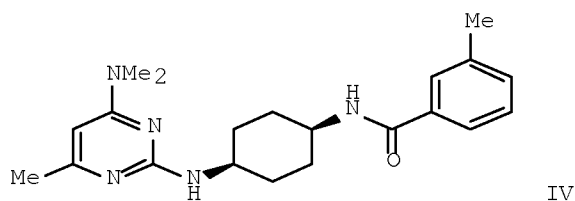
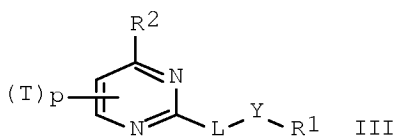
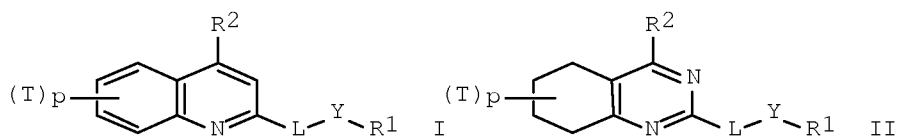
Relative stereochemistry.



L58 ANSWER 21 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:875032 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:350191
TITLE: Preparation of quinoline, tetrahydroquinazoline, and
pyrimidine derivatives as MCH antagonist for treatment
of CNS disorders
INVENTOR(S): Sekiguchi, Yoshinori; Kanuma, Kosuke; Omodera,
Katsunori; Busujima, Tsuyoshi; Tran, Thuy-Anh; Han,
Sangdon; Casper, Martin; Kramer, Bryan A.; Semple,
Graeme; Zou, Ning
PATENT ASSIGNEE(S): Taisho Pharmaceutical Co. Ltd., Japan
SOURCE: Eur. Pat. Appl., 586 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1464335	A2	20041006	EP 2004-7651	20040330
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
EP 1464335	A2	20041006	EP 2004-7651	20040330
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
PRIORITY APPLN. INFO.:			US 2003-458530P	P 20030331
			US 2003-495911P	P 20030819
			US 2003-510186P	P 20031009
			US 2003-530360P	P 20031216
			EP 2004-7651	A 20040330

GI



- AB Title compds. I, II, and III [wherein R1 = (un)substituted (cyclo)alkyl, (cyclo)alkenyl, alkynyl, aryl; R2 = H, halo, OH, carboxy, carbamoyl, amino, (un)substituted alkyl, alkoxy; T = independently H, halo, OH, carboxy, carbamoyl, amino, cyano, NO₂, alkenyl, alkynyl, cycloalkyl, (un)substituted alkyl, alkoxy; p = 0-5; L = aminocycloalkylideneamino, etc.; Y = bond, CH₂, CO₂, OCO, SO₂, CO, CS, CONH, CSNH, etc.; with provisos; and pharmaceutically acceptable salts, hydrates, or solvates thereof] were prepared as antagonists of melanin concentrating hormone (MCH), an endogenous ligand of G-protein coupled receptors (GPCRs). Examples include solution and solid phase general synthetic methods and phys. data for nearly 3400 invention compds. In addition, all exemplified compds. were assayed using high throughput functional screening to detect intracellular Ca²⁺ concns. for accessing GPCR activation. For instance, reaction of 2,4-dichloro-6-methylpyrimidine with dimethylamine gave 2-chloro-4-(dimethylamino)-6-methylpyrimidine (40%), which was coupled with cis-(4-aminocyclohexyl)carbamic acid tert-Bu ester (60%). Deprotection (72%), amidation, and workup provided the benzamide IV•TFA. The latter demonstrated MCH antagonist activity with an IC₅₀ value of 7.6 nM. Thus, pharmaceutical compns. comprising I are useful for the prophylaxis or treatment of improving memory function, sleeping and arousal, anxiety, depression, mood disorders, seizure, obesity, diabetes, appetite and eating disorders, cardiovascular disease, hypertension, dyslipidemia, myocardial infarction, binge eating disorders including bulimia, anorexia, mental disorders including manic depression, schizophrenia, delirium, dementia, stress, cognitive disorders, attention deficit disorder, substance abuse disorders, and dyskinesias including Parkinson's disease, epilepsy, and addiction (no data). This is part II of three in a series covering the patent.
- IT 771545-69-8P 771551-46-3P 771554-02-0P,
 2-(3,4-Dichlorophenylamino)-N-[cis-4-[(quinolin-2-yl)amino]cyclohexyl]acetamide dihydrochloride 771554-83-7P,
 2-(3,4-Dichlorophenylamino)-N-[cis-4-[(4-methylquinolin-2-yl)amino]cyclohexyl]acetamide dihydrochloride
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (melanin-concentrating hormone antagonist; preparation of quinolines,

10/598508

quinazolines,

and pyrimidines as melanin-concentrating hormone antagonist for treatment of

CNS disorders)

RN 771545-69-8 ZCAPLUS

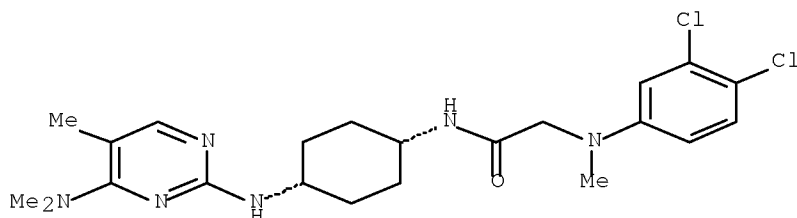
CN Acetamide, 2-[(3,4-dichlorophenyl)methylamino]-N-[cis-4-[[4-(dimethylamino)-5-methyl-2-pyrimidinyl]amino]cyclohexyl]-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 771545-68-7

CMF C22 H30 Cl2 N6 O

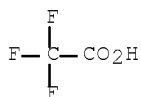
Relative stereochemistry.



CM 2

CRN 76-05-1

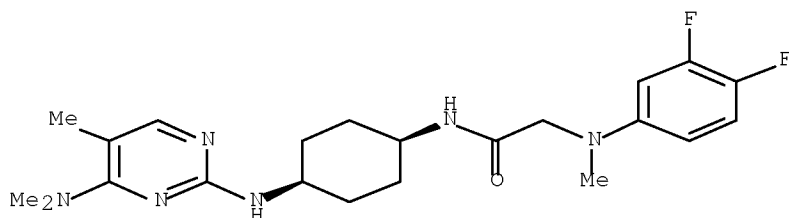
CMF C2 H F3 O2



RN 771551-46-3 ZCAPLUS

CN Acetamide, 2-[(3,4-difluorophenyl)methylamino]-N-[cis-4-[[4-(dimethylamino)-5-methyl-2-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

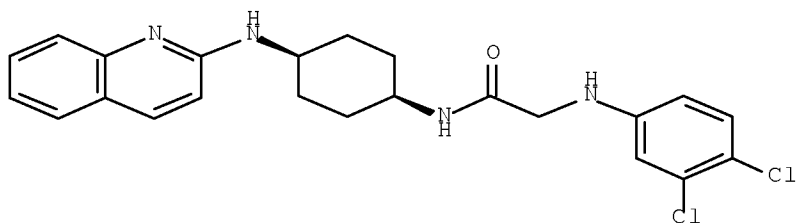


10/598508

RN 771554-02-0 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-[cis-4-(2-quinolinylamino)cyclohexyl]-, hydrochloride (1:2) (CA INDEX NAME)

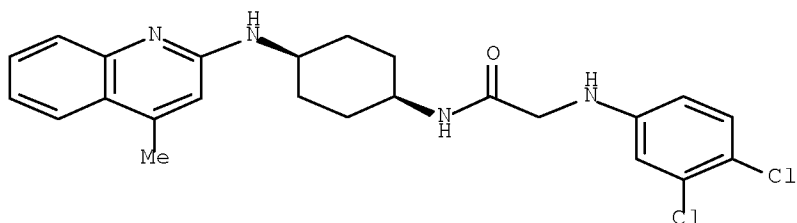
Relative stereochemistry.



RN 771554-83-7 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-[cis-4-[(4-methyl-2-quinolinyl)amino]cyclohexyl]-, hydrochloride (1:2) (CA INDEX NAME)

Relative stereochemistry.



L58 ANSWER 22 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:756686 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:277494

TITLE: Preparation of diaryl substituted pyrrolidinones and pyrrolones having activity at 5-HT_{2c} receptor

INVENTOR(S): Damiani, Federica; Hamprecht, Dieter; Micheli, Fabrizio; Pasquarello, Alessandra; Tedesco, Giovanna

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 32 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078718	A1	20040916	WO 2004-EP1843	20040224

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1599445 A1 20051130 EP 2004-713874 20040224

EP 1599445 B1 20080402

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

JP 2006519241 T 20060824 JP 2006-504465 20040224

AT 391121 T 20080415 AT 2004-713874 20040224

US 20060205788 A1 20060914 US 2005-548118 20050902

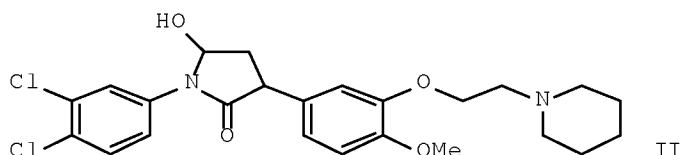
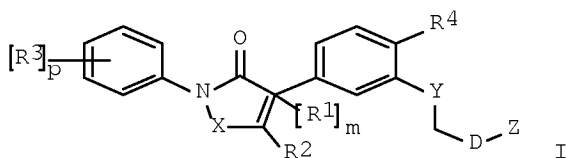
PRIORITY APPLN. INFO.:

GB 2003-5024 A 20030305

WO 2004-EP1843 W 20040224

OTHER SOURCE(S): MARPAT 141:277494

GI



AB The title compds. [I; R1 = H, F, Cl, OH, alkyl, cycloalkyl, cycloalkyloxy, alkoxy or haloalkoxy; m = 0-1; R2 = H, halo, CN, NO2, alkyl, cycloalkyl, cycloalkyloxy, haloalkyl, alkoxy, haloalkoxy, alkylthio, amino, mono- or dialkylamino or an N-linked 4-7 membered heterocyclic group; X = CH2CH2, CH:CH, (CH2)3, C(CH3)2, CH:CHCH2, CH2CH:CH or CHR5 (wherein R5 = H, halo, OH, CN, NO2, alkyl, cycloalkyl, cycloalkyloxy, haloalkyl, alkoxy, haloalkoxy or alkylthio); R3 = halo, CN, alkyl, cycloalkyl, cycloalkyloxy, alkoxy, alkylthio, OH, NH2, mono- or dialkylamino, etc.; p = 0-3; R4 = H, halo, OH, CN, NO2, alkyl, alkanoyl, cycloalkyl, cycloalkyloxy, haloalkyl, alkoxy, haloalkoxy, alkylthio, amino, mono- or dialkylamino or an N-linked 4-7 membered heterocyclic group; Y = O, S, CH2 or NR10 (wherein R10 = H, alkyl); D = a single bond, CH2, (CH2)2 or CH:CH; Z = NR11R12 (where R11 and R12 = H, alkyl, (un)substituted N-linked or C-linked 4-7 membered heterocyclic group)] and their pharmaceutically acceptable salts, useful in treating, for example, depression and anxiety, were prepared. E.g., a multi-step synthesis of II, was given. All exemplified compds. I were tested for their affinity for the 5-HT2c receptor, and were found to have pKi values >5.8. The pharmaceutical composition comprising the compound I is disclosed.

IT 103038-71-7P 758707-87-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

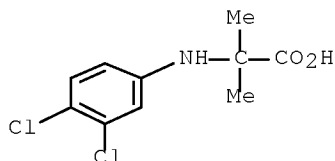
10/598508

(Reactant or reagent)

(preparation of diaryl substituted pyrrolidinones and pyrrolones having activity at 5-HT_{2c} receptor)

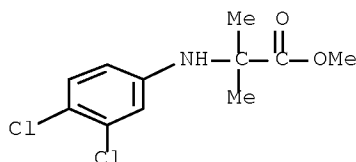
RN 103038-71-7 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-2-methyl- (CA INDEX NAME)



RN 758707-87-8 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-2-methyl-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 23 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:702514 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:392610

TITLE: Synthesis and properties of symmetrical and asymmetrical phthalocyanines with DL-leucine fragments

AUTHOR(S): Naumov, A. O.; Kudrik, E. V.; Shaposhnikov, G. P.

CORPORATE SOURCE: Ivanovo State University of Chemistry and Technology, Ivanovo, 153460, Russia

SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2004), 40(4), 469-474

CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:392610

AB Nucleophilic substitution of the nitro group in 4-nitrophthalonitrile by the DL-leucine fragment yields N-(3,4-dicyanophenyl)-DL-leucine possessing a chiral site. This product was used to synthesize new sym. and asym. phthalocyanines.

IT 850015-32-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

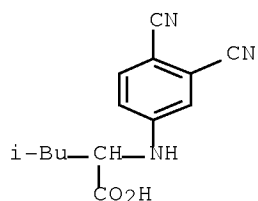
(synthesis and properties of sym. and asym. phthalocyanines with

10/598508

DL-leucine fragments)

RN 850015-32-6 ZCAPLUS

CN Leucine, N-(3,4-dicyanophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 24 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:298673 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:314225

TITLE: Synthesis and evaluation of certain pyrazolines and related compounds for their antitubercular, antibacterial and antifungal activities

AUTHOR(S): Chetan, B. P.; Sreenivas, M. T.; Bhat, A. R.

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, K.L.E.S.'s College of Pharmacy, Belgaum, 590 010, India

SOURCE: Indian Journal of Heterocyclic Chemistry (2004), 13(3), 225-228

CODEN: IJCHEI; ISSN: 0971-1627

PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:314225

AB New pyrazoline derivs. of 3-chloro-4-fluoro-aniline derived from both by reacting through chloroacetyl chloride with pyrazoline and through Mannich reaction were synthesized. The compds. were screened for antitubercular, antibacterial and antifungal activities in vitro. Title compds. showed antitubercular activity at 10 µg and 100 µg per mL concentration level. The compds. were moderately active as antibacterial agents against *S. aureus* and *E. coli* compared to the standard. The compds. did not show antifungal activity even at 50 µg per disk concentration level.

IT 766538-15-2P 766538-16-3P 766538-17-4P

766538-18-5P 766538-20-9P 845959-82-2P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

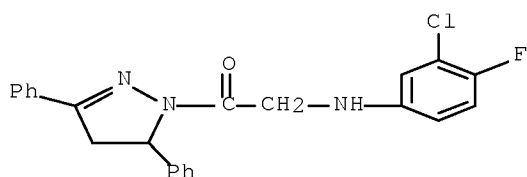
BIOL (Biological study); PREP (Preparation)

(synthesis of pyrazolines via cyclocondensation and Mannich reactions and evaluation for their antitubercular, antibacterial, and antifungal activities)

RN 766538-15-2 ZCAPLUS

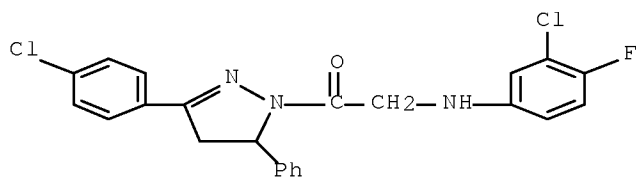
CN Ethanone, 2-[(3-chloro-4-fluorophenyl)amino]-1-(4,5-dihydro-3,5-diphenyl-1H-pyrazol-1-yl)- (CA INDEX NAME)

10/598508



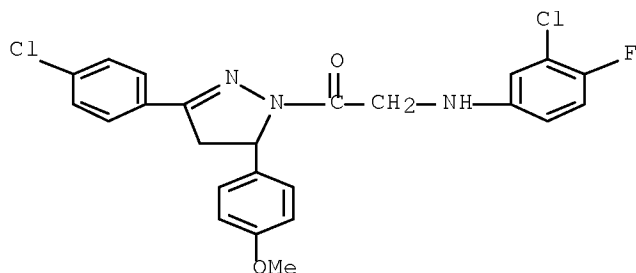
RN 766538-16-3 ZCAPLUS

CN Ethanone, 2-[(3-chloro-4-fluorophenyl)amino]-1-[3-(4-chlorophenyl)-4,5-dihydro-5-phenyl-1H-pyrazol-1-yl]- (CA INDEX NAME)



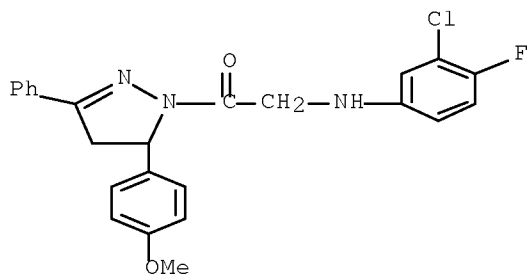
RN 766538-17-4 ZCAPLUS

CN Ethanone, 2-[(3-chloro-4-fluorophenyl)amino]-1-[3-(4-chlorophenyl)-4,5-dihydro-5-(4-methoxyphenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

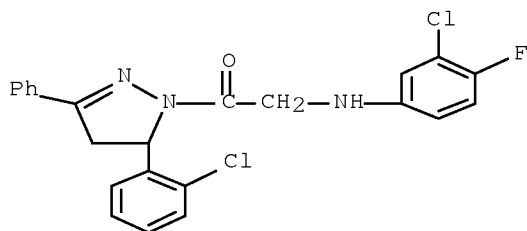


RN 766538-18-5 ZCAPLUS

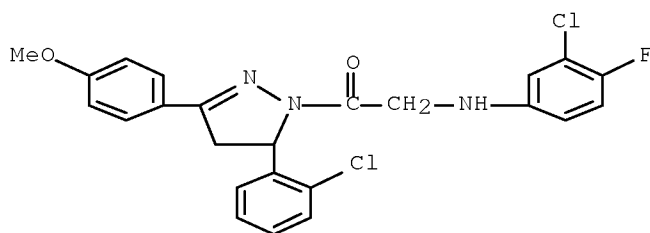
CN Ethanone, 2-[(3-chloro-4-fluorophenyl)amino]-1-[4,5-dihydro-5-(4-methoxyphenyl)-3-phenyl-1H-pyrazol-1-yl]- (CA INDEX NAME)



RN 766538-20-9 ZCAPLUS
 CN Ethanone, 2-[(3-chloro-4-fluorophenyl)amino]-1-[5-(2-chlorophenyl)-4,5-dihydro-3-phenyl-1H-pyrazol-1-yl]- (CA INDEX NAME)



RN 845959-82-2 ZCAPLUS
 CN Ethanone, 2-[(3-chloro-4-fluorophenyl)amino]-1-[5-(2-chlorophenyl)-4,5-dihydro-3-(4-methoxyphenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 25 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:692088 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:323474

TITLE: Synthesis and biological evaluation of a novel phenyl-substituted sydnone series as potential antitumor agents

AUTHOR(S): Dunkley, Christopher S.; Thoman, Charles J.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, 19104, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(17), 2899-2901

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:323474

AB A series of compds. containing an N-(4-substituted 3-nitrophenyl)sydnone moiety with potential antitumor activity was prepared based on active analogs.

10/598508

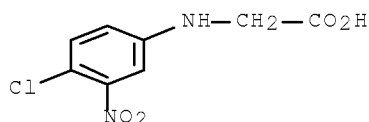
The rationale behind the design of these compds. is presented along with the 4-step synthetic route to the derivs. Out of the six novel compds., the N-(4-fluoro-3-nitrophenyl) derivative has an improved activity against all three tested cell lines as compared to the earlier leads.

IT 89938-35-2 613683-77-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and antitumor activity of N-(4-substituted 3-nitrophenyl)sydnonones)

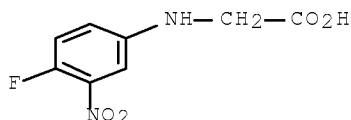
RN 89938-35-2 ZCAPLUS

CN Glycine, N-(4-chloro-3-nitrophenyl)- (CA INDEX NAME)



RN 613683-77-5 ZCAPLUS

CN Glycine, N-(4-fluoro-3-nitrophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 26 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:35360 ZCAPLUS Full-text

DOCUMENT NUMBER: 138:90080

TITLE: Preparation of heterocyclic compounds and their use for inhibiting β -amyloid peptide release

INVENTOR(S): Thorsett, Eugene D.; Porter, Warren J.; Nissen, Jeffrey S.; Latimer, Lee H.; Audia, James E.; Droste, James

PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; Eli Lilly and Company
SOURCE: U.S., 99 pp.

CODEN: USXXAM

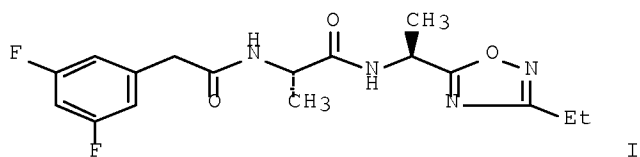
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 6506782	B1	20030114	US 1998-32019	19980227
US 20030130188	A1	20030710	US 2002-246558	20020919
US 6849650	B2	20050201		
PRIORITY APPLN. INFO.:			US 1998-32019	A3 19980227
OTHER SOURCE(S):	MARPAT	138:90080		
GI				



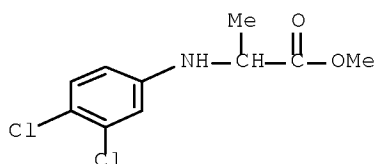
AB Disclosed are modified heterocyclic di- and tripeptide analogs which inhibit β -amyloid peptide release and/or its synthesis and, accordingly, have utility in treating Alzheimer's disease. Compds. of formula $R_1NHCHR_2(CONHCHR_6)pCONHCHR_5C(:NR_4)R_4$ [$R_1 = H$ or acyl; $R_2, R_5, R_6 =$ (un)substituted alk(en)(yn)yl, cycloalkyl, (hetero)aryl, heterocyclyl; $p = 0$ or 1; R_3 and R_4 combine to form a heterocyclic ring, which may be substituted] are claimed. Also disclosed are pharmaceutical compns. comprising a compound which inhibits β -amyloid peptide release and/or its synthesis as well as methods for treating Alzheimer's disease both prophylactically and therapeutically with such pharmaceutical compns. Title compds., e.g. I, were prepared in a multistep synthesis and inhibited β -amyloid peptide production by at least 30% as compared to control.

IT 83442-68-6P 83442-80-2P 106146-57-0P
 106146-58-1P 106146-59-2P 208339-09-7P
 208339-10-0P 208339-11-1P 208339-12-2P
 208339-13-3P 208339-14-4P 208339-15-5P
 208339-16-6P 208339-17-7P 208339-18-8P
 208339-19-9P 208339-21-3P 208339-22-4P
 208339-23-5P 208339-25-7P 208339-30-4P
 208339-31-5P 208339-32-6P 208339-33-7P
 208339-38-2P 208339-39-3P 208339-40-6P
 208339-48-4P 209995-94-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of heterocyclic compds. and their use for inhibiting
 β -amyloid peptide release)

RN 83442-68-6 ZCAPLUS

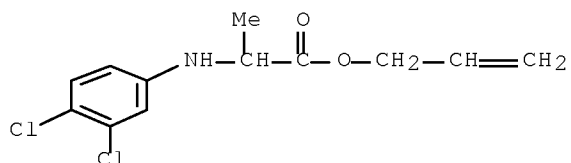
CN Alanine, N-(3,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)



RN 83442-80-2 ZCAPLUS

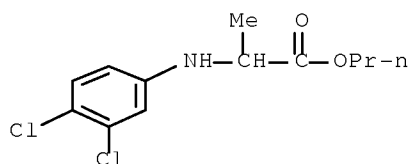
CN Alanine, N-(3,4-dichlorophenyl)-, 2-propenyl ester (9CI) (CA INDEX NAME)

10/598508



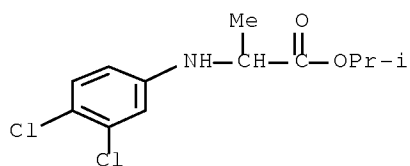
RN 106146-57-0 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, propyl ester (CA INDEX NAME)



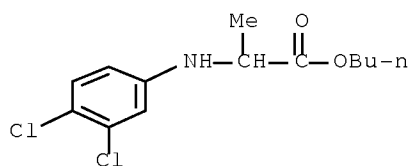
RN 106146-58-1 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 1-methylethyl ester (CA INDEX NAME)



RN 106146-59-2 ZCAPLUS

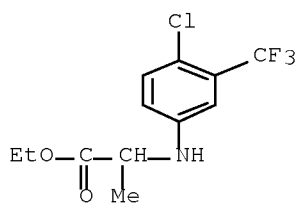
CN Alanine, N-(3,4-dichlorophenyl)-, butyl ester (CA INDEX NAME)



RN 208339-09-7 ZCAPLUS

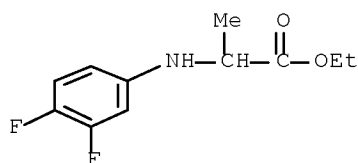
CN Alanine, N-[4-chloro-3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

10/598508



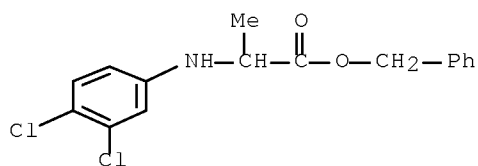
RN 208339-10-0 ZCAPLUS

CN Alanine, N-(3,4-difluorophenyl)-, ethyl ester (CA INDEX NAME)



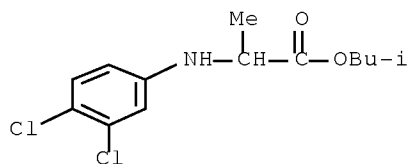
RN 208339-11-1 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, phenylmethyl ester (CA INDEX NAME)



RN 208339-12-2 ZCAPLUS

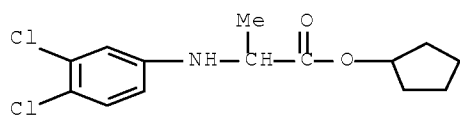
CN Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-13-3 ZCAPLUS

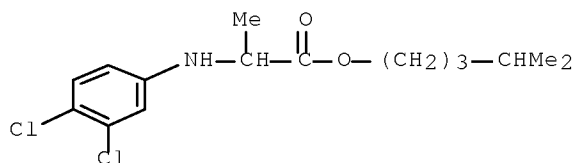
CN Alanine, N-(3,4-dichlorophenyl)-, cyclopentyl ester (CA INDEX NAME)

10/598508



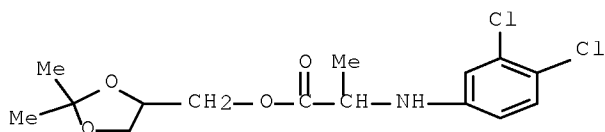
RN 208339-14-4 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 4-methylpentyl ester (CA INDEX NAME)



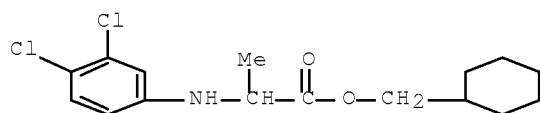
RN 208339-15-5 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, (2,2-dimethyl-1,3-dioxolan-4-yl)methyl ester (CA INDEX NAME)



RN 208339-16-6 ZCAPLUS

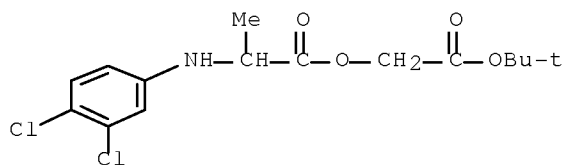
CN Alanine, N-(3,4-dichlorophenyl)-, cyclohexylmethyl ester (CA INDEX NAME)



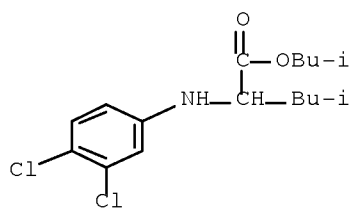
RN 208339-17-7 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-(1,1-dimethylethoxy)-2-oxoethyl ester (CA INDEX NAME)

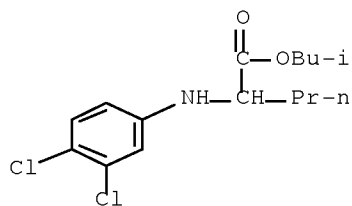
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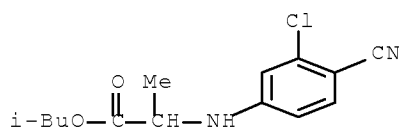
RN 208339-18-8 ZCAPLUS
CN Leucine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-19-9 ZCAPLUS
CN Norvaline, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



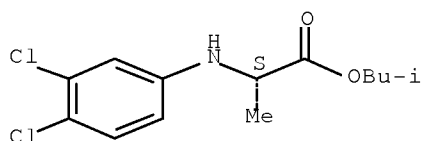
RN 208339-21-3 ZCAPLUS
CN Alanine, N-(3-chloro-4-cyanophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-22-4 ZCAPLUS
CN L-Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)

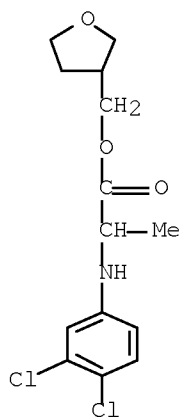
Absolute stereochemistry.

10/598508



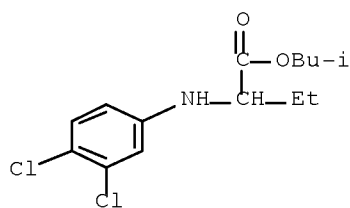
RN 208339-23-5 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, (tetrahydro-3-furanyl)methyl ester (CA INDEX NAME)



RN 208339-25-7 ZCAPLUS

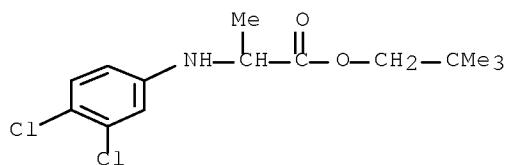
CN Butanoic acid, 2-[(3,4-dichlorophenyl)amino]-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-30-4 ZCAPLUS

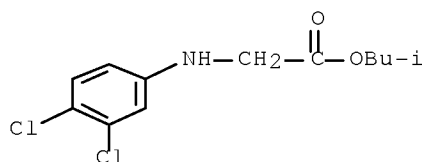
CN Alanine, N-(3,4-dichlorophenyl)-, 2,2-dimethylpropyl ester (CA INDEX NAME)

10/598508



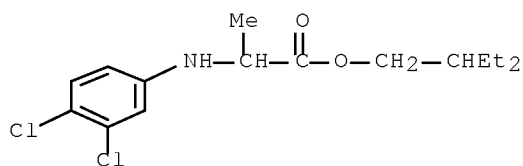
RN 208339-31-5 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



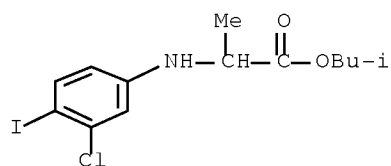
RN 208339-32-6 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-ethylbutyl ester (CA INDEX NAME)



RN 208339-33-7 ZCAPLUS

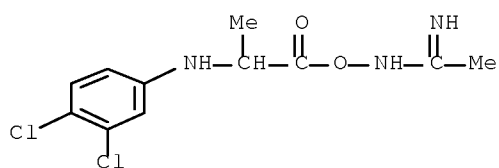
CN Alanine, N-(3-chloro-4-iodophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-38-2 ZCAPLUS

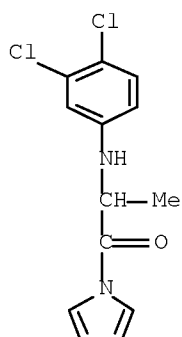
CN Ethanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)

10/598508



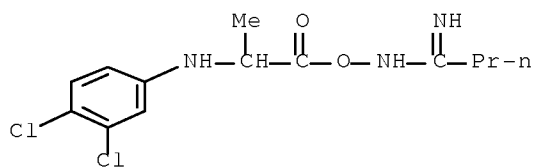
RN 208339-39-3 ZCAPLUS

CN 1H-Pyrrole, 1-[2-[(3,4-dichlorophenyl)amino]-1-oxopropyl]- (9CI) (CA INDEX NAME)



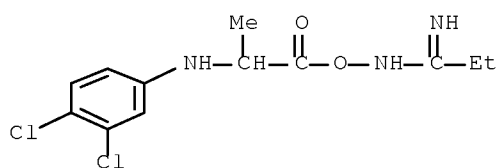
RN 208339-40-6 ZCAPLUS

CN Butanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)



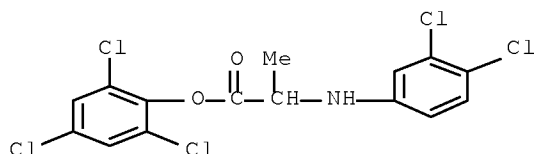
RN 208339-48-4 ZCAPLUS

CN Propanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)



10/598508

RN 209995-94-8 ZCAPLUS
CN Alanine, N-(3,4-dichlorophenyl)-, 2,4,6-trichlorophenyl ester (CA INDEX NAME)



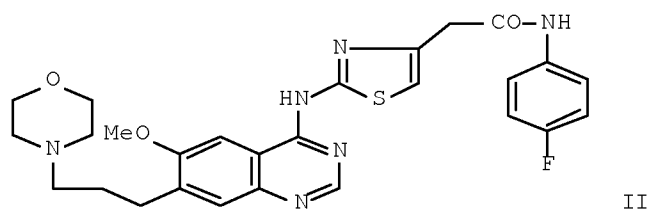
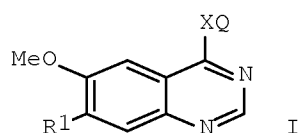
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 27 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:10468 ZCAPLUS Full-text
DOCUMENT NUMBER: 136:85826
TITLE: Preparation of substituted quinazoline derivatives and their use as inhibitors of AURORA-2 kinase
INVENTOR(S): Mortlock, Andrew; Jung, Frederic
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 249 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002000649	A1	20020103	WO 2001-SE1450	20010621
WO 2002000649	A9	20070920		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG, AP, EA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, EP, OA				
CA 2412592	A1	20020103	CA 2001-2412592	20010621
EP 1299381	A1	20030409	EP 2001-944061	20010621
EP 1299381	B1	20080507		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001011754	A	20030429	BR 2001-11754	20010621
HU 2003001236	A2	20031028	HU 2003-1236	20010621
JP 2004501914	T	20040122	JP 2002-505773	20010621
CN 1496364	A	20040512	CN 2001-814620	20010621
EE 200200715	A	20040816	EE 2002-715	20010621
NZ 522696	A	20040827	NZ 2001-522696	20010621
RU 2283311	C2	20060910	RU 2003-102389	20010621
AT 394102	T	20080515	AT 2001-944061	20010621

10/598508

IN 2002MN01598	A	20041211	IN 2002-MN1598	20021112
ZA 2002009412	A	20040219	ZA 2002-9412	20021119
MX 2002PA11974	A	20040906	MX 2002-PA11974	20021203
BG 107376	A	20030930	BG 2002-107376	20021211
NO 2002006010	A	20021213	NO 2002-6010	20021213
US 20030187002	A1	20031002	US 2002-311916	20021216
US 6919338	B2	20050719		
US 20060046987	A1	20060302	US 2005-70057	20050302
PRIORITY APPLN. INFO.:			EP 2000-401842	A 20000628
			WO 2001-SE1450	W 20010621
			US 2002-311916	A1 20021216
OTHER SOURCE(S):	MARPAT 136:85826			
GI				



AB The title compds. [I; X = O, S, S:O, SO₂, NR; R = H, C1-6alkyl; R1 = OCH₃, 3-(4-morpholinyl)propoxy, N-methylpiperidine-4-ylmethoxy, 3-(N-methylpiperazine-4-yl)propoxy, 3-(pyrrolidine-1-yl)propoxy, (CH₃)₂N(CH₂)₃O, etc.; Q = (un)substituted 5-membered heteroarom.], pharmaceutically acceptable salts, in vivo hydrolysable esters, and amides are prepared as AURORA-2 kinase inhibitors in warm blooded animals. The title compds. together with pharmaceutical compns. containing them are also described and claimed. Thus, the title compound II was prepared and tested in vitro for the ability to arrest MCF7 cells in specific phases of the cell cycle.

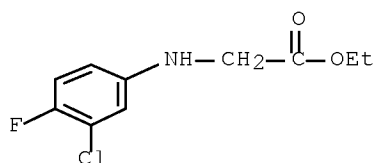
IT 2344-98-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of quinazoline derivs. and use as inhibitors of AURORA-2 kinase)

RN 2344-98-1 ZCAPLUS

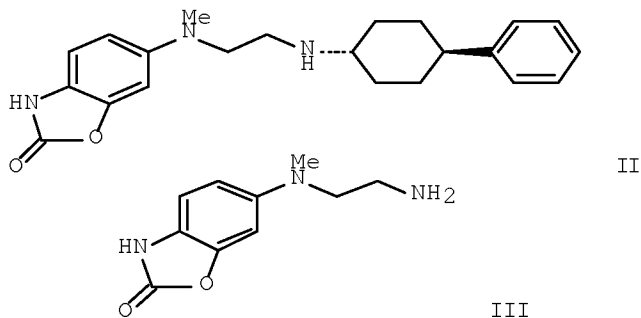
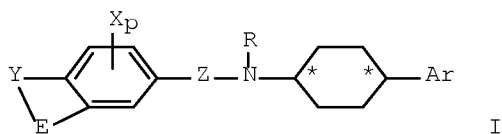
CN Glycine, N-(3-chloro-4-fluorophenyl)-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 28 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:904121 ZCAPLUS Full-text
 DOCUMENT NUMBER: 136:37615
 TITLE: Preparation of bicyclic cyclohexylamines and their use as NMDA receptor antagonists
 INVENTOR(S): Deorazio, Russell Joseph; Nikam, Sham Shridhar; Scott, Ian Leslie; Sherer, Brian Alan; Wise, Lawrence David
 PATENT ASSIGNEE(S): Warner-Lambert Company, USA
 SOURCE: PCT Int. Appl., 62 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001094321	A1	20011213	WO 2001-US15605	20010514
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2407164	A1	20011213	CA 2001-2407164	20010514
AU 2001063130	A	20011217	AU 2001-63130	20010514
EP 1292581	A1	20030319	EP 2001-937387	20010514
EP 1292581	B1	20050810		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003535851	T	20031202	JP 2002-501871	20010514
BR 2001011267	A	20031216	BR 2001-11267	20010514
AT 301642	T	20050815	AT 2001-937387	20010514
ES 2243500	T3	20051201	ES 2001-937387	20010514
MX 2002PA10503	A	20030310	MX 2002-PA10503	20021024
US 20030232810	A1	20031218	US 2002-297263	20021203
US 6683101	B2	20040127		
PRIORITY APPLN. INFO.:			US 2000-209485P	P 20000606
			WO 2001-US15605	W 20010514
OTHER SOURCE(S):			MARPAT 136:37615	
GI				



AB Heterocycle-substituted cyclohexylamines I (Ar = (un)substituted aryl with halo, OH or O-alkyl, SH, CN, NO₂, NH-alkyl, OAc or CF₃ group or with 5 to 14 atom heteroaryl with 1 to 2 heteroatoms of N, O, or S; E-Y = OC(O)NH, HNC(O)NH, C(O)CH₂NH, CH₂S(O)NH, SCH₂C(O)NH, etc.; X = independently selected from H, halogen, NO₂, CN, CF₃, etc.; p = 0-2; Z = (CH₂)_n, CO, S(O) where n = 1-6, etc.; R = H, alkyl, C(O)(ara)alkyl, OH- or NH-alkyl, alkenylalkyl, etc.; * = cis- or trans- isomer) and their pharmaceutically acceptable salts were prepared I are antagonists of NMDA receptor channel complexes useful for treating cerebral vascular disorders such as, for example, cerebral ischemia, cardiac arrest, stroke, and Parkinson's disease. Thus II was prepared in 17% yield from sarcosine Et ester HCl and 5-fluoro-2-nitrophenol via III which reacted with 4-phenylcyclohexanone in 2-propanol, THF, Et₃N and NaBH₄. In 6-OHDA lesioned rats the min. ED of II required to produce a statistically significant increase in total contraversive rotations compared to rats receiving L-DOPA only was 1.0 μM .

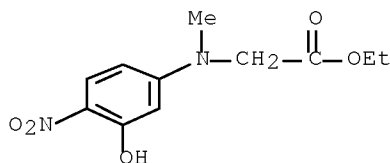
IT 380198-13-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bicyclic cyclohexylamines and their use as NMDA receptor antagonists)

RN 380198-13-0 ZCAPLUS

CN Glycine, N-(3-hydroxy-4-nitrophenyl)-N-methyl-, ethyl ester (CA INDEX NAME)



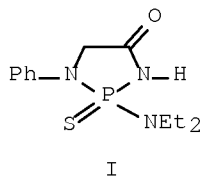
REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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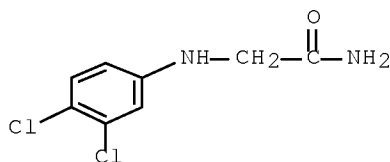
L58 ANSWER 29 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:646342 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 135:344556
TITLE: Synthesis of 1,3,2-diazaphospholidin-4-one-2-selenide
(sulfide) derivatives and their biological activity
AUTHOR(S): Deng, Sheng-Lou; Chen, Ru-Yu; Yang, Xiu-Feng
CORPORATE SOURCE: Institute of Elemento-Organic Chemistry, State Key
Laboratory of Elemento-Organic Chemistry, NanKai
University, Tianjin, 300071, Peop. Rep. China
SOURCE: Yingyong Huaxue (2001), 18(8), 647-650
CODEN: YIHUED; ISSN: 1000-0518
PUBLISHER: Yingyong Huaxue Bianji Weiyuanhui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 135:344556
GI



AB A series of five-membered phosphorus heterocycles, e.g. I, were synthesized by reacting tris(diethylamino)phosphine with α -aminoacetamides. Their structures were characterized by elemental anal. and ^1H NMR, some by MS, IR and ^{31}P NMR as well. The preliminary bioassays show that these compds. possess good selective herbicidal activity and some of them also have had antiviral and fungicidal activities.

IT 117919-59-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization with tris(diethylamino)phosphine)

RN 117919-59-2 ZCAPLUS
CN Acetamide, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



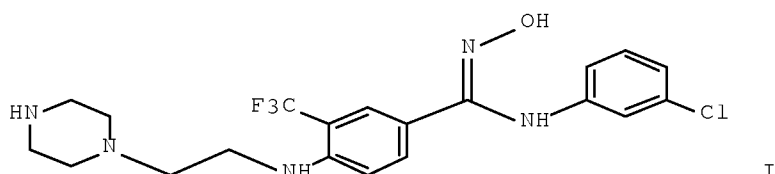
L58 ANSWER 30 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:526050 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 135:107149
TITLE: Synthesis, antibacterial activity and RNA polymerase

10/598508

inhibition of phenylamidine derivs.
 INVENTOR(S): Li, Leping; Chen, Xiaoqui; Fan, Pingchen; Mihalic, Jeffrey Thomas; Cutler, Serena
 PATENT ASSIGNEE(S): Tularik Inc., USA
 SOURCE: PCT Int. Appl., 104 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001051456	A2	20010719	WO 2001-US1219	20010112
WO 2001051456	A3	20011220		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2397575	A1	20010719	CA 2001-2397575	20010112
US 20020045749	A1	20020418	US 2001-759633	20010112
US 6780858	B2	20040824		
EP 1246795	A2	20021009	EP 2001-914329	20010112
EP 1246795	B1	20071031		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003519676	T	20030624	JP 2001-551838	20010112
AT 376996	T	20071115	AT 2001-914329	20010112
ES 2293980	T3	20080401	ES 2001-914329	20010112
US 20040235911	A1	20041125	US 2004-877408	20040625
US 7053234	B2	20060530		
US 20060270651	A1	20061130	US 2006-344111	20060201
US 7148259	B1	20061212		
PRIORITY APPLN. INFO.:			US 2000-175892P	P 20000113
			US 2001-759633	A1 20010112
			WO 2001-US1219	W 20010112
			US 2004-877408	A3 20040625

OTHER SOURCE(S): MARPAT 135:107149
 GI



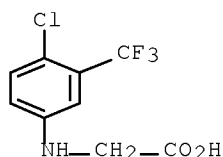
10/598508

AB Synthesis of hydroxyamidines, e.g. (I) and related compds. are disclosed which are suitable as antibacterial agents by their inhibition of RNA polymerase. Antibacterial activity against *S. aureus* and *E. coli* are given.

IT 782-61-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis, antibacterial activity and RNA polymerase inhibition of phenyl- and heterocyclylhydroxyamidine derivs.)

RN 782-61-6 ZCAPLUS

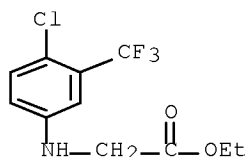
CN Glycine, N-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



IT 2345-03-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis, antibacterial activity and RNA polymerase inhibition of phenyl- and heterocyclylhydroxyamidine derivs.)

RN 2345-03-1 ZCAPLUS

CN Glycine, N-[4-chloro-3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



L58 ANSWER 31 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:105630 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 134:290324

TITLE: Functional gamma-secretase inhibitors reduce beta-amyloid peptide levels in brain

AUTHOR(S): Dovey, H. F.; John, V.; Anderson, J. P.; Chen, L. Z.; De Saint Andrieu, P.; Fang, L. Y.; Freedman, S. B.; Folmer, B.; Goldbach, E.; Holsztynska, E. J.; Hu, K. L.; Johnson-Wood, K. L.; Kennedy, S. L.; Kholodenko, D.; Knops, J. E.; Latimer, L. H.; Lee, M.; Liao, Z.; Lieberburg, I. M.; Motter, R. N.; Mutter, L. C.; Nietz, J.; Quinn, K. P.; Sacchi, K. L.; Seubert, P. A.; Shopp, G. M.; Thorsett, E. D.; Tung, J. S.; Wu, J.; Yang, S.; Yin, C. T.; Schenk, D. B.; May, P. C.; Altstiel, L. D.; Bender, M. H.; Boggs, L. N.; Britton, T. C.; Clemens, J. C.; Czilli, D. L.; Dieckman-McGinty, D. K.; Droste, J. J.; Fuson, K. S.; Gitter, B. D.; Hyslop, P. A.; Johnstone, E. M.; Li, W-Y.; Little, S. P.; Mabry, T. E.; Miller, F. D.; Ni,

B.; Nissen, J. S.; Porter, W. J.; Potts, B. D.; Reel, J. K.; Stephenson, D.; Su, Y.; Shipley, L. A.; Whitesitt, C. A.; Yin, T.; Audia, J. E.
 CORPORATE SOURCE: Elan Pharmaceuticals, Inc., South San Francisco, CA, 94080, USA
 SOURCE: Journal of Neurochemistry (2001), 76(1), 173-181
 CODEN: JONRA9; ISSN: 0022-3042
 PUBLISHER: Blackwell Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Converging lines of evidence implicate the beta-amyloid peptide (A β) as causative in Alzheimer's disease. We describe a novel class of compds. that reduce A β production by functionally inhibiting γ -secretase, the activity responsible for the carboxy-terminal cleavage required for A β production. These mols. are active in both 293 HEK cells and neuronal cultures, and exert their effect upon A β production without affecting protein secretion, most notably in the secreted forms of the amyloid precursor protein (APP). Oral administration of one of these compds., N-[N-(3,5-difluorophenacetyl)-L-alanyl]-S-phenylglycine t-Bu ester, to mice transgenic for human APPV717F reduces brain levels of A β in a dose-dependent manner within 3 h. These studies represent the first demonstration of a reduction of brain A β in vivo. Development of such novel functional γ -secretase inhibitors will enable a clin. examination of the A β hypothesis that A β peptide drives the neuropathol. observed in Alzheimer's disease.

IT ~~208339-22-4~~

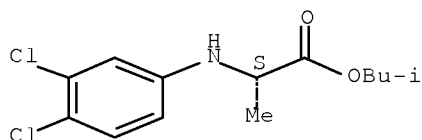
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(functional gamma-secretase inhibitors reduce beta-amyloid peptide levels in brain)

RN 208339-22-4 ZCAPLUS

CN L-Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 32 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:133714 ZCAPLUS Full-text

DOCUMENT NUMBER: 132:180871

TITLE: Preparation of hepatitis C inhibitory tripeptides

INVENTOR(S): Llinas-Brunet, Montse; Bailey, Murray D.; Cameron, Dale; Faucher, Anne-Marie; Ghio, Elise; Goudreau, Nathalie; Halmos, Teddy; Poupert, Marc-Andre; Rancourt, Jean; Tsantrizos, Youla S.; Wernic, Dominik M.; Simoneau, Bruno

PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE: PCT Int. Appl., 168 pp.

10/598508

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

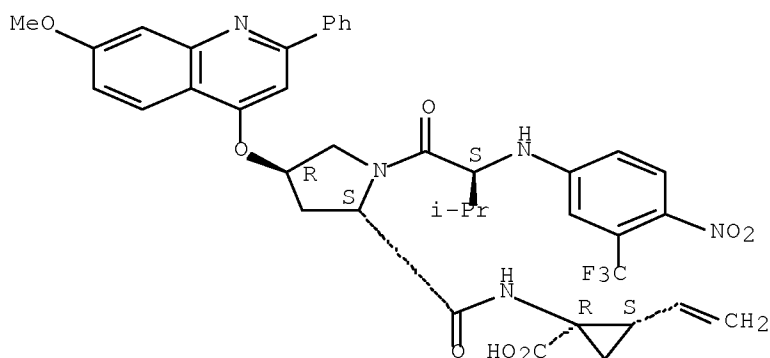
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000009543	A2	20000224	WO 1999-CA736	19990809
WO 2000009543	A3	20000525		
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6323180	B1	20011127	US 1999-368866	19990805
CA 2338946	A1	20000224	CA 1999-2338946	19990809
CA 2445938	A1	20000224	CA 1999-2445938	19990809
AU 9952731	A	20000306	AU 1999-52731	19990809
AU 769738	B2	20040205		
BR 9913646	A	20010605	BR 1999-13646	19990809
EP 1105413	A2	20010613	EP 1999-938084	19990809
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
TR 200100432	T2	20010921	TR 2001-432	19990809
CN 1323316	A	20011121	CN 1999-810550	19990809
HU 2001005144	A2	20020429	HU 2001-5144	19990809
HU 2001005144	A3	20021128		
TR 200200129	T2	20020621	TR 2002-129	19990809
JP 2002522554	T	20020723	JP 2000-564993	19990809
EE 200100081	A	20020815	EE 2001-81	19990809
NZ 510396	A	20040227	NZ 1999-510396	19990809
TW 250165	B	20060301	TW 1999-88113586	19990809
CN 101143892	A	20080319	CN 2007-10140740	19990809
US 6268207	B1	20010731	US 2000-660030	20000912
US 6329379	B1	20011211	US 2000-675398	20000929
US 6329417	B1	20011211	US 2000-703751	20001101
MX 2001PA01423	A	20000821	MX 2001-PA1423	20010207
IN 2001MN00127	A	20050304	IN 2001-MN127	20010207
BG 105232	A	20011130	BG 2001-105232	20010208
HR 2001000102	A1	20020228	HR 2001-102	20010208
NO 2001000683	A	20010402	NO 2001-683	20010209
US 20020016442	A1	20020207	US 2001-827976	20010406
US 6420380	B2	20020716		
US 20020037998	A1	20020328	US 2001-849057	20010504
US 6410531	B2	20020625		
US 6534523	B1	20030318	US 2002-91293	20020305
IN 2007MN00706	A	20070720	IN 2007-MN706	20070511
PRIORITY APPLN. INFO.:			US 1998-95931P	P 19980810
			US 1999-132386P	P 19990504
			US 1999-368866	A3 19990805
			CA 1999-2338946	A 19990809
			CN 1999-810550	A3 19990809
			WO 1999-CA736	W 19990809
			IN 2001-MN127	A3 20010207
			US 2001-849057	A1 20010504
OTHER SOURCE(S):	MARPAT 132:180871			

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB Peptides I [B = H, (un)substituted aryl, aralkyl, heterocyclyl, or alkylheterocyclyl, acyl R4CO, carboxylate R4O2C, amide R4NR5CO, thioamide R4NR5C(S), or sulfonyl group R4SO2, where R4 = (un)substituted alkyl, cycloalkyl, cycloalkoxy, amino, aralkyl, or heterocyclyl, with proviso that R4 ≠ cycloalkoxy for amides or thioamides; R5, Y = H, alkyl; R3 = (un)substituted alkyl, cycloalkyl, or alkylcycloalkyl; R2 = (un)substituted cycloalkyl-, aryl-, aralkyl-, or heterocyclylmethyl, -amino, -oxy, or -thio; R1 = H; alkyl, cycloalkyl, alkenyl, or alkynyl, all optionally substituted with halogen] or their racemates, diastereoisomers, and optical isomers were prepared as hepatitis C virus (HCV) inhibitory tripeptides. Thus, compound II was prepared via peptide coupling reactions in solution and showed IC50 < 0.5 μM in the recombinant HCV NS3 protease/NS4A cofactor peptide radiometric assay.
- IT 259216-33-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of hepatitis C inhibitory tripeptides)
- RN 259216-33-6 ZCAPLUS
- CN Cyclopropanecarboxylic acid, N-[4-nitro-3-(trifluoromethyl)phenyl]-L-valyl-(4R)-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-L-prolyl-1-amino-2-ethenyl-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 33 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:62622 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 132:122929
 TITLE: Method for preparation of optically active
 N-(3-phthalimidophenyl)amino acid derivative and its
 intermediates and herbicide containing the same as
 active ingredient
 INVENTOR(S): Natsume, Fumitsugu; Ono, Fumihiko; Tanaka, Takeshi;
 Hosokawa, Akemi; Hikido, Mitsuru
 PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.

10/598508

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000026414	A	20000125	JP 1998-197178	19980713
PRIORITY APPLN. INFO.:			JP 1998-197178	19980713
OTHER SOURCE(S):	CASREACT 132:122929; MARPAT 132:122929			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

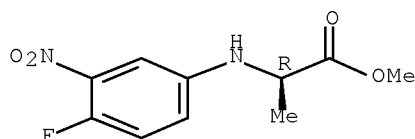
AB The title compds. [I; A = O, S, NH, C1-4 alkylimino; R = H, C1-6 alkyl, C2-6 alkenyl, C3-6 cycloalkyl, C1-4 haloalkyl, C2-5 cyanoalkyl, C2-6 alkoxyalkyl, alkylthioalkyl, or alkylsulfonylalkyl, C3-7 acyloxyalkyl, C3-8 alkoxycarbonylalkyl, (un)substituted Ph, (un)substituted phenyl-C1-3 alkyl, (un)substituted 3- to 6-membered heterocyclyl containing 1-2 O, S, and/or N, C1-3 alkyl substituted by (un)substituted 3- to 6-membered heterocyclyl containing 1-2 O, S, and/or N; or when A = NH or C1-4 alkylimino, R together with A optionally form a 5- to 6-membered heterocyclyl containing 1-2 N and 0-1; R1 = C1-4 alkyl; X = halo; Y = H, halo; Z = H, C1-3 alkyl, halo] are prepared via imidation of N-(3-aminophenyl)amino acids (II; A, R, R1, X, Y = same as above) with phthalic anhydride (III; Z = same as above). Thus, 7.2 g phthalic anhydride and 10.0 g Me (R)-2-[(5-amino-2- chloro-4- fluorophenyl)amino]propanoate (preparation given) were dissolved in 20 AcOH and heated to reflux with stirring for 1.5 h to give the title compound (IV) in 79% yield. IV at 5 g/ha postemergence controlled 100% Galium spurium and 91-99% Stellaria media.

IT 256229-89-7F, Methyl (R)-2-[(3-nitro-4- fluorophenyl)amino]propanoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active N-(3-phthalimidophenyl)amino acid derivative as herbicide and its intermediates)

RN 256229-89-7 ZCAPLUS

CN D-Alanine, N-(4-fluoro-3-nitrophenyl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



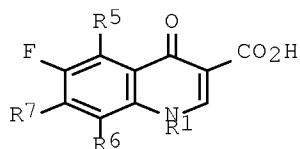
L58 ANSWER 34 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:465689 ZCAPLUS Full-text
DOCUMENT NUMBER: 131:87832
TITLE: Preparation of quinolonecarboxylates from

10/598508

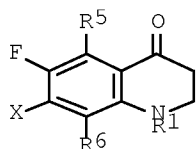
oxotetrahydroquinolines.
 INVENTOR(S): Egle, Ian; Karimian, Khashayar; Xin, Tao; Leung-Toung, C. S. H. Regis; Tam, Tim Fat; Lei, Bo
 PATENT ASSIGNEE(S): Apotex Inc., Can.
 SOURCE: Can. Pat. Appl., 51 pp.
 CODEN: CPXXEB
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2199645	A1	19980911	CA 1997-2199645	19970311
CA 2199645	C	19990629		
US 5914401	A	19990622	US 1998-37982	19980311
PRIORITY APPLN. INFO.:			CA 1997-2199645	A 19970311
OTHER SOURCE(S):		CASREACT 131:87832; MARPAT 131:87832		

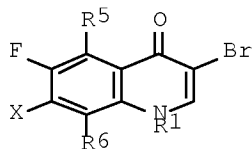
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I



II



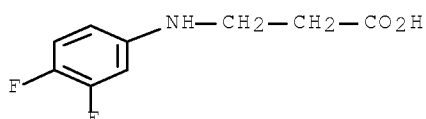
III

AB Title compds. [I; R1 = alkyl, cycloalkyl; R6 = H, alkyl, alkoxy, halo; R6R1 = OCH2CHR4; R4 = H, alkyl; R5 = H; R7 = NRR1; R, R1 = H, alkyl, pyrrolidinyl, piperazinyl, prolyl, morpholinyl, piperidinyl, (substituted) piperazinyl, etc.], were prepared by bromination of tetrahydroquinolones (II; R1, R5, R5 as above; X undefined) to give bromo derivs. (III; variables as above) followed by treatment with R7H to give (III X = R7; other variables as above), cyanation, and hydrolysis. Norfloxacin and ciprofloxacin were prepared by the claimed method.

IT 229324-10-1F, 3-(3,4-Difluorophenylamino)propionic acid
 229324-11-2F 229324-20-3F
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of quinolonecarboxylates from oxotetrahydroquinolines)

RN 229324-10-1 ZCAPLUS

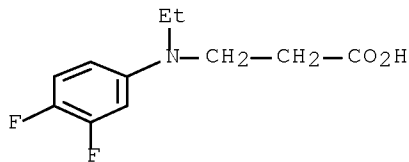
CN β-Alanine, N-(3,4-difluorophenyl)- (CA INDEX NAME)



10/598508

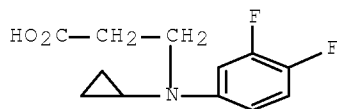
RN 229324-11-2 ZCAPLUS

CN β -Alanine, N-(3,4-difluorophenyl)-N-ethyl- (CA INDEX NAME)



RN 229324-20-3 ZCAPLUS

CN β -Alanine, N-cyclopropyl-N-(3,4-difluorophenyl)- (CA INDEX NAME)



L58 ANSWER 35 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:436242 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 131:228632

TITLE: Synthesis of some new 1-ethyl-6-fluoro-2,3-dihydro-4-oxo-7-(substituted aryloxy/arylamino)quinolines as antibacterial agents

AUTHOR(S): Saravanan, J.; Murthy, S. Narasimha; Manjunath, K. S.
CORPORATE SOURCE: M.S. Ramaiah college of pharmacy, Bangalore, 560 054, India

SOURCE: Indian Drugs (1999), 36(3), 192-195

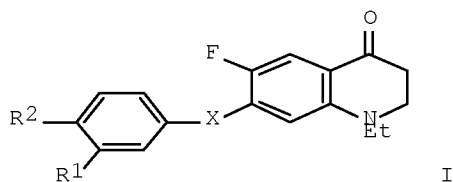
CODEN: INDRBA; ISSN: 0019-462X

PUBLISHER: Indian Drug Manufacturers' Association

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

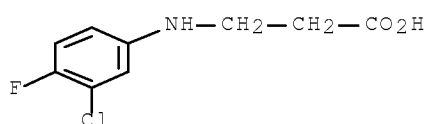


AB 3-Chloro-4-fluoroaniline with acrylonitrile gave the cyanoethylated product, which, on alkaline hydrolysis, gave the corresponding carboxylic acid. This acid, on cyclization with polyphosphoric acid, yielded the corresponding dihydroquinolinone, which, on treatment with Et iodide and subsequently with various substituted phenols and substituted primary arylamines in the presence of phase transfer catalysts, yielded the title compds. (I; R1 = H, Me, Br; R2 = H, Cl, MeO, NO2; X = O, NH). I were screened for antibacterial activity.

IT 114417-22-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of)

RN 114417-22-0 ZCAPLUS

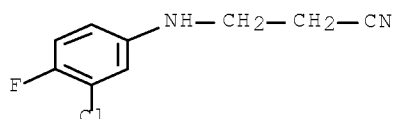
CN β -Alanine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)



IT 244070-75-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrolysis of)

RN 244070-75-5 ZCAPLUS

CN Propanenitrile, 3-[(3-chloro-4-fluorophenyl)amino]- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 36 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:348897 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 131:129970

TITLE: Synthesis of some new biologically active thiadiazolotriazinones. Part II

AUTHOR(S): Holla, B. Shivarama; Sarojini, B. K.; Shridhara, K.; Antony, Georgy

CORPORATE SOURCE: Department of Post Graduate Studies and Research in Chemistry, Mangalore University, Mangalagangothri, 574 199, India

SOURCE: Farmaco (1999), 54(3), 149-151
 CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

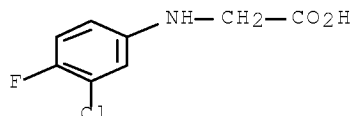
10/598508

AB 4-Amino-6-phenyl/methyl-3-mercapto-1,2,4-triazin-5(4H)-ones are condensed with an aromatic carboxylic acid, aryloxyacetic acid or anilinoacetic acid, to yield 7-substituted-3-phenyl/methyl-4H-1,3,4-thiadiazolo[2,3-c]-1,2,4-triazin-4-ones. POCl₃ was used as a cyclizing agent. All the synthesized compds. are screened for their antibacterial activities against *S. aureus*, *E. coli*, *P. aeruginosa* and *G. bacillus*.

IT 83442-58-4, 3-Chloro-4-fluoroanilinoacetic acid
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of and bactericidal activity of thiadiazolotriazinones)

RN 83442-58-4 ZCAPLUS

CN Glycine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 37 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:233912 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 130:252373

TITLE: Preparation and formulation of O-containing heterocyclic derivatives as cysteine protease inhibitors

INVENTOR(S): Usui, Yoshihiro; Masuda, Hirokazu; Ando, Naoko; Nakao, Akira; Ando, Ryoichi; Yoshii, Narihiko; Saito, Ken-ichi

PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan

SOURCE: PCT Int. Appl., 115 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

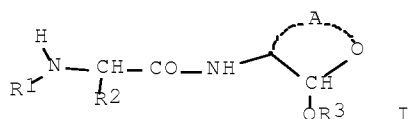
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9916761	A1	19990408	WO 1998-JP4420	19980930
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 11171881	A	19990629	JP 1998-277586	19980930
PRIORITY APPLN. INFO.:			JP 1997-266034	A 19970930
OTHER SOURCE(S):	MARPAT 130:252373			

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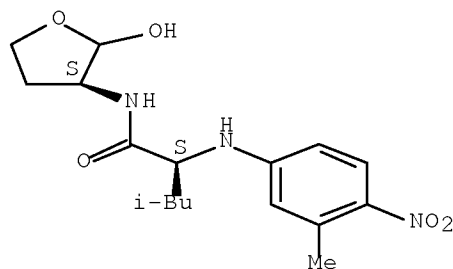
AB The title compds. I [R1 represents optionally substituted C6-14 aryl or an optionally substituted heterocycle residue; R2 represents hydrogen or C1-10 alkyl optionally substituted by C6-14 aryl; R3 represents hydrogen or R4CO (R4 represents C1-10 alkyl); and A represents C1-3 alkylene optionally substituted by C1-3 alkyl] are prepared I are useful as cysteine protease inhibitors excellent in oral absorbability, migration to tissues, and can easily pass through the cell membrane, etc. (3S)-3-[(S)-2-(4,6- dimethoxy-2-pyrimidinyl)amino-4-methylvaleryl-amino]-2-tetrahydrofuranol in vitro showed IC50 of 1.27 μ M against calpain.

IT 221683-23-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of O-containing heterocyclic derivs. as cysteine protease inhibitors)

RN 221683-23-4 ZCAPLUS

CN Pentanamide, 4-methyl-2-[(3-methyl-4-nitrophenyl)amino]-N-[(3S)-tetrahydro-2-hydroxy-3-furanyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 38 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:192896 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 130:325116

TITLE: Studies on some N-bridged heterocycles derived from bis[4-amino-5-mercapto-1,2,4-triazol-3-yl]alkanes

AUTHOR(S): Holla, B. Shivarama; Gonsalves, Richard; Shenoy, Shalini

CORPORATE SOURCE: Department of P.G. Studies and Research in Chemistry, Mangalore University, Mangalagangothri, 574199, India

SOURCE: Farmaco (1998), 53(8-9), 574-578
 CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of bis[4-amino-5-mercapto-1,2,4-triazol-3-yl]alkanes have been synthesized and were converted into bis[1,2,4-triazolo[3,4-b]-1,3,4-thiadiazol-4-yl]alkanes. Some of the newly synthesized compds. were screened for their antibacterial properties and exhibited activity with MIC in the range 3-12.5 μ g/mL.

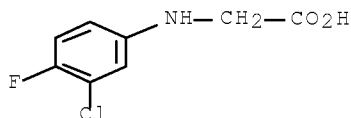
10/598508

IT 83442-58-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and antibacterial activity of
bis[triazolothiadiazolyl]alkanes)

RN 83442-58-4 ZCAPLUS

CN Glycine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 39 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:178216 ZCAPLUS Full-text

DOCUMENT NUMBER: 130:237851

TITLE: Synthesis of N-phenylvaline derivatives under phase
transfer catalysis

AUTHOR(S): Galin, F. Z.; Rakhimov, R. G.; Tolstikov, G. A.

CORPORATE SOURCE: Institute of Organic Chemistry, Russian Academy of
Sciences, Ufa, Russia

SOURCE: Russian Journal of Organic Chemistry (Translation of
Zhurnal Organicheskoi Khimii) (1998), 34(6), 899

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 4,5,2-R1,R2,R3-C6H2NHCH(CHMe2)CO2H (R1, R2, R3 = H, F, H; F, F, H; H, CF3, Cl;
CF3, H, H) were prepared by reaction of fluoroarylamines with Me α -
bromoisovalerate under phase transfer catalysis (50% solution of KOH,
triethylbutylammonium chloride, 60°).

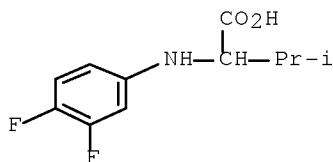
IT 221302-26-7F

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of N-phenylvaline derivs. under phase transfer catalysis)

RN 221302-26-7 ZCAPLUS

CN Valine, N-(3,4-difluorophenyl)- (CA INDEX NAME)



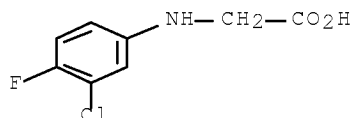
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 40 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:634389 ZCAPLUS Full-text

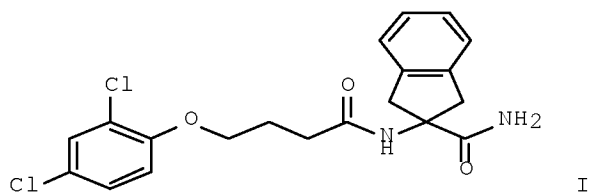
10/598508

DOCUMENT NUMBER: 129:316198
TITLE: Synthesis of some new biologically active
thiadiazolotriazinones
AUTHOR(S): Holla, B. Shivarama; Sarojini, B. K.; Gonsalves,
Richard
CORPORATE SOURCE: Department of Post-Graduate Studies and Research in
Chemistry, Mangalore University, Mangalagangothri, 574
199, India
SOURCE: Farmaco (1998), 53(6), 395-398
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 4-Amino-6-arylmethyl-3-mercapto-1,2,4-triazin-5(4H)-ones are condensed with
aromatic carboxylic acids, aryloxyacetic acids and anilinoacetic acids to
yield 7-substituted-3-arylmethyl-4H-1,3,4-thiadiazolo[2,3-c]-1,2,4- triazin-4-
ones. Phosphorus oxychloride is used as cyclizing agent. The products have
antibacterial activity similar to that of furacin.
IT 83442-58-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bactericidal thiadiazolotriazinones)
RN 83442-58-4 ZCAPLUS
CN Glycine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 41 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:630372 ZCAPLUS Full-text
DOCUMENT NUMBER: 129:331032
TITLE: Exploring structure-activity relationships around the
phosphomannose isomerase inhibitor AF14049 via
combinatorial synthesis
AUTHOR(S): Bhandari, Ashok; Jones, David G.; Schullek, John R.;
Vo, Kham; Schunk, Caryn A.; Tamanaha, Lisa L.; Chen,
Dawn; Yuan, Zhengyu; Needels, Michael C.; Gallop, Mark
A.
CORPORATE SOURCE: Affymax Research Institute, Palo Alto, CA, 94304, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998),
8(17), 2303-2308
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Phosphomannose isomerase (PMI) has been shown by genetic methods to be an essential enzyme in fungal cell wall biosynthesis. The PMI inhibitor AF14049 (I) was discovered as an unanticipated side product from high-throughput library screening against the enzyme from *C. albicans*. Solid-phase synthetic methods were developed and a series of libraries and discrete analogs synthesized to explore SAR around AF14049.

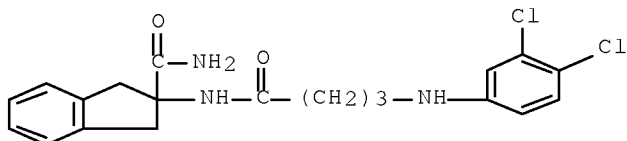
IT 215094-91-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(structure-activity of aminoindanecarboxamide phosphomannose isomerase inhibitor AF14049 via combinatorial synthesis)

RN 215094-91-0 ZCAPLUS

CN 1H-Indene-2-carboxamide, 2-[[4-[(3,4-dichlorophenyl)amino]-1-oxobutyl]amino]-2,3-dihydro- (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 42 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:608608 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:245485

TITLE: Preparation of heterocyclic compounds and their use for inhibiting β -amyloid peptide release

INVENTOR(S): Thorsett, Eugene D.; Porter, Warren J.; Nissen, Jeffrey S.; Latimer, Lee H.; Audia, James E.; Droste, James J.

PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; Eli Lilly & Co.

SOURCE: PCT Int. Appl., 392 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

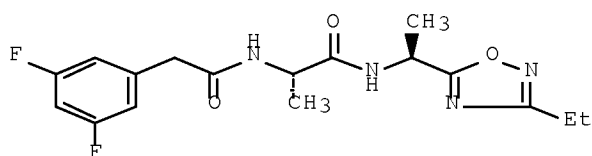
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
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CA 2278674 A1 19980903 CA 1998-2278674 19980227
AU 9866622 A 19980918 AU 1998-66622 19980227
EP 968198 A1 20000105 EP 1998-908637 19980227
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BR 9807876 A 20000229 BR 1998-7876 19980227
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JP 2001513107 T 20010828 JP 1998-537732 19980227
NO 9904016 A 19991018 NO 1999-4016 19990819
PRIORITY APPLN. INFO.: US 1997-808263 A1 19970228
WO 1998-US3373 W 19980227
OTHER SOURCE(S): MARPAT 129:245485
GI



AB Disclosed are modified heterocyclic di- and tripeptide analogs which inhibit β -amyloid peptide release and/or its synthesis, and, accordingly, have utility in treating Alzheimer's disease. Also disclosed are pharmaceutical compns. comprising a compound which inhibits β -amyloid peptide release and/or its synthesis as well as methods for treating Alzheimer's disease both prophylactically and therapeutically with such pharmaceutical compns. Title compds., e.g. I, were prepared in a multistep synthesis and inhibited β -amyloid peptide production by at least 30% as compared to control.

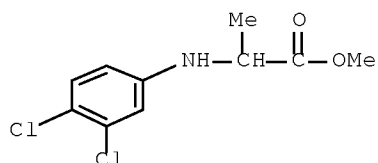
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208339-48-4P 209995-94-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

10/598508

(preparation of heterocyclic compds. and their use for inhibiting
β-amyloid peptide release)

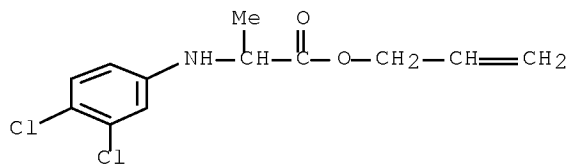
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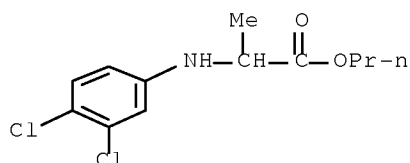
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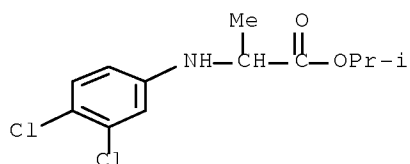
RN 106146-57-0 ZCAPLUS

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RN 106146-58-1 ZCAPLUS

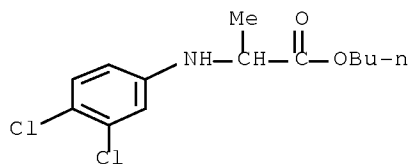
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10/598508

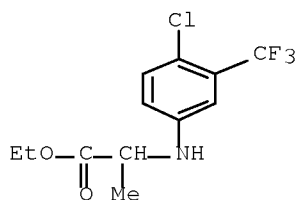
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CN Alanine, N-(3,4-dichlorophenyl)-, butyl ester (CA INDEX NAME)



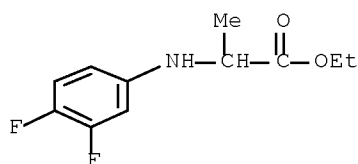
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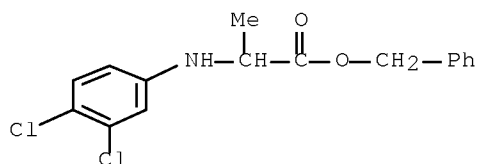
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CN Alanine, N-(3,4-difluorophenyl)-, ethyl ester (CA INDEX NAME)



RN 208339-11-1 ZCAPLUS

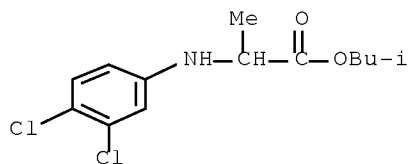
CN Alanine, N-(3,4-dichlorophenyl)-, phenylmethyl ester (CA INDEX NAME)



10/598508

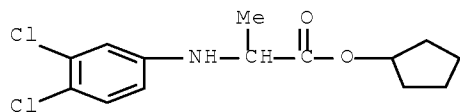
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CN Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



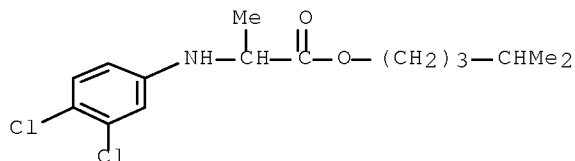
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CN Alanine, N-(3,4-dichlorophenyl)-, cyclopentyl ester (CA INDEX NAME)



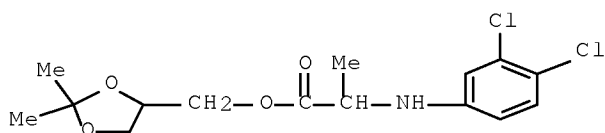
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CN Alanine, N-(3,4-dichlorophenyl)-, 4-methylpentyl ester (CA INDEX NAME)



RN 208339-15-5 ZCAPLUS

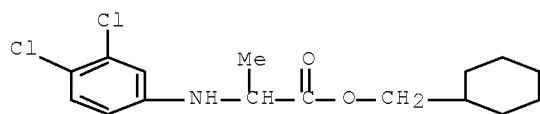
CN Alanine, N-(3,4-dichlorophenyl)-, (2,2-dimethyl-1,3-dioxolan-4-yl)methyl ester (CA INDEX NAME)



RN 208339-16-6 ZCAPLUS

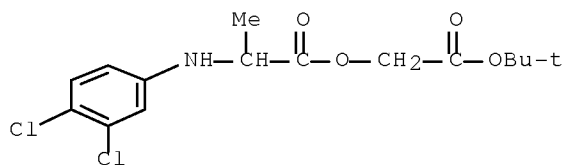
CN Alanine, N-(3,4-dichlorophenyl)-, cyclohexylmethyl ester (CA INDEX NAME)

10/598508



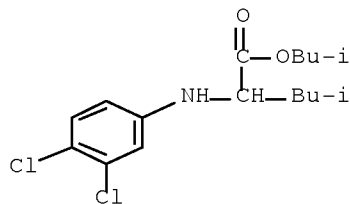
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CN Alanine, N-(3,4-dichlorophenyl)-, 2-(1,1-dimethylethoxy)-2-oxoethyl ester
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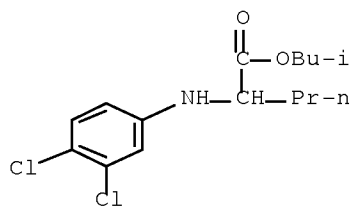
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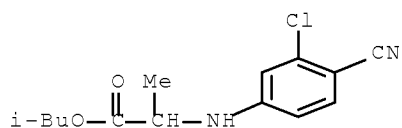
CN Norvaline, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-21-3 ZCAPLUS

CN Alanine, N-(3-chloro-4-cyanophenyl)-, 2-methylpropyl ester (CA INDEX NAME)

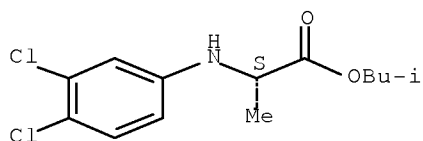
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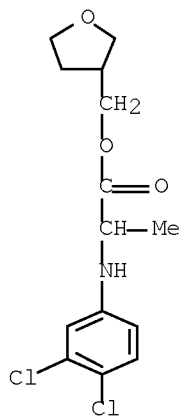
CN L-Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



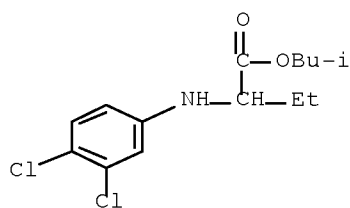
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CN Alanine, N-(3,4-dichlorophenyl)-, (tetrahydro-3-furanyl)methyl ester (CA INDEX NAME)



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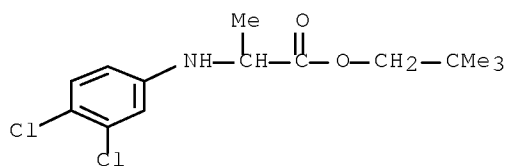
CN Butanoic acid, 2-[(3,4-dichlorophenyl)amino]-, 2-methylpropyl ester (CA INDEX NAME)



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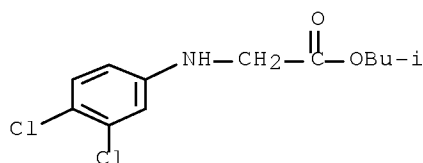
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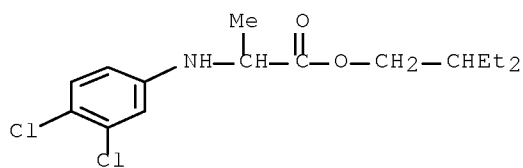
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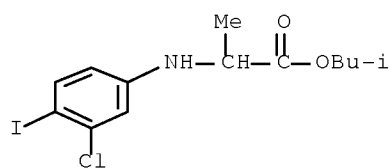
RN 208339-32-6 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-ethylbutyl ester (CA INDEX NAME)



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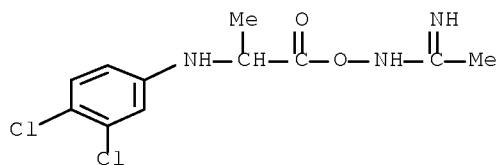
CN Alanine, N-(3-chloro-4-iodophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



10/598508

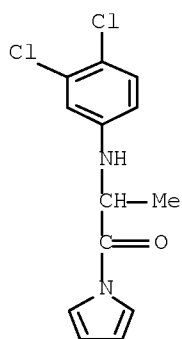
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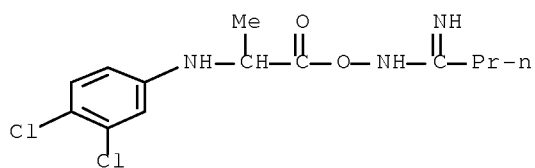
RN 208339-39-3 ZCAPLUS

CN 1H-Pyrrole, 1-[2-[(3,4-dichlorophenyl)amino]-1-oxopropyl]- (9CI) (CA INDEX NAME)



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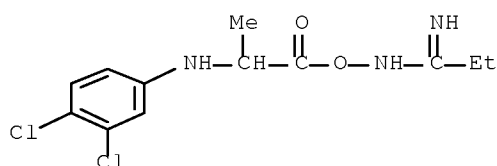
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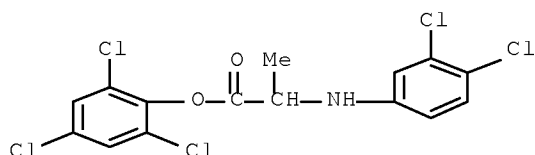
RN 208339-48-4 ZCAPLUS

CN Propanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)

10/598508



RN 209995-94-8 ZCAPLUS
CN Alanine, N-(3,4-dichlorophenyl)-, 2,4,6-trichlorophenyl ester (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 43 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:479505 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 129:122870
TITLE: Preparation of cycloalkyl, lactam, lactone and related compounds for inhibiting β -amyloid peptide release and/or its synthesis
INVENTOR(S): Wu, Jing; Tung, Jay S.; Thorsett, Eugene D.; Pleiss, Michael A.; Nissen, Jeffrey S.; Neitz, Jeffrey; Latimer, Lee H.; John, Varghese; Freedman, Stephen; Britton, Thomas C.; Audia, James E.; Reel, Jon K.; Mabry, Thomas E.; Dressman, Bruce A.; Cwi, Cynthia L.; Droste, James J.; Henry, Steven S.; Mcdaniel, Stacey L.; Scott, William Leonard; Stucky, Russell D.; Porter, Warren J.
PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; Eli Lilly & Co.
SOURCE: PCT Int. Appl., 889 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9828268	A2	19980702	WO 1997-US22986	19971222
WO 9828268	A3	19981008		
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NZ 335583	A	20010330	NZ 1997-335583	19971222
CN 1616432	A	20050518	CN 2004-10057888	19971222
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OTHER SOURCE(S): MARPAT 129:122870

AB Disclosed are compds. R1ZmNHnCHpR2C(X)R3 [R1 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, or cycloalkenyl or aryl, heteroaryl, or heterocyclic; R2 and R3 form a cycloalkyl, cycloalkenyl, heterocyclic, substituted cycloalkyl, or substituted cycloalkenyl ring which is optionally fused; X = oxo, thioxo, hydroxyl, thiol, or hydro; Y = CHR4CONH where R4 = (un)substituted alkyl, alkenyl, or alkynyl or cycloalkyl, aryl, heteroaryl, or heterocyclic; Z is TCX'X''CO where T is a bond, O, S, NR5 (R5 = H, acyl, alkyl, aryl, or heteroaryl), X' and X'' are H, OH, or F or X'X'' = oxo; m, p = 0, 1; n = 0, 1, 2] which inhibit β -amyloid peptide release and/or its

10/598508

synthesis, and, accordingly, have utility in treating Alzheimer's disease. Thus, 3-[[N'-(3,4- methylenedioxyphenylacetyl)-L-alaninyl]amino]-2,3-dihydro-1-methyl-5- phenyl-1H-1,4-benzodiazepin-2-one was prepared by coupling of 3-(L-alaninylamino)-2,3-dihydro-1-methyl-5-phenyl-1H-1,4-benzodiazepin-2- one with 3,4-methylenedioxyphenylacetic acid.

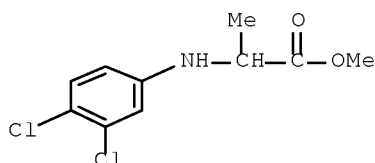
IT 83442-68-6P 209995-94-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cycloalkyl, lactam, lactone and related compds. for inhibiting β -amyloid peptide release and/or its synthesis)

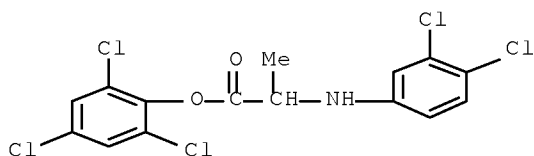
RN 83442-68-6 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)



RN 209995-94-8 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2,4,6-trichlorophenyl ester (CA INDEX NAME)



IT 83442-80-2P 106146-57-0P 106146-58-1P
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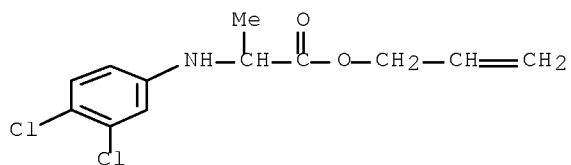
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of cycloalkyl, lactam, lactone and related compds. for inhibiting β -amyloid peptide release and/or its synthesis)

RN 83442-80-2 ZCAPLUS

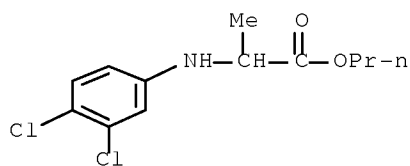
CN Alanine, N-(3,4-dichlorophenyl)-, 2-propenyl ester (9CI) (CA INDEX NAME)

10/598508



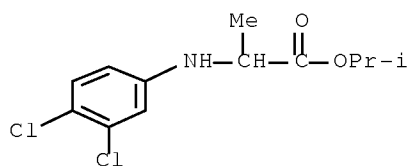
RN 106146-57-0 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, propyl ester (CA INDEX NAME)



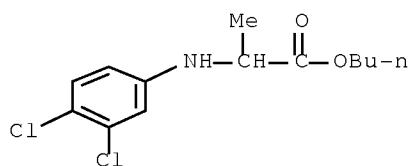
RN 106146-58-1 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 1-methylethyl ester (CA INDEX NAME)



RN 106146-59-2 ZCAPLUS

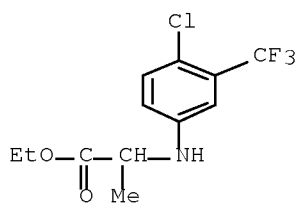
CN Alanine, N-(3,4-dichlorophenyl)-, butyl ester (CA INDEX NAME)



RN 208339-09-7 ZCAPLUS

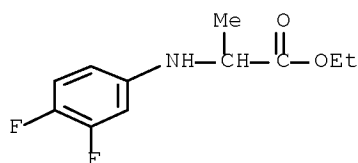
CN Alanine, N-[4-chloro-3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

10/598508



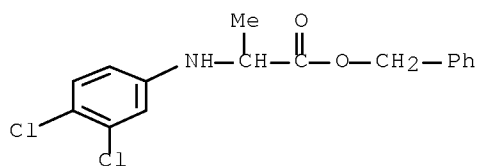
RN 208339-10-0 ZCAPLUS

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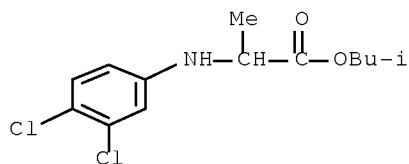
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CN Alanine, N-(3,4-dichlorophenyl)-, phenylmethyl ester (CA INDEX NAME)



RN 208339-12-2 ZCAPLUS

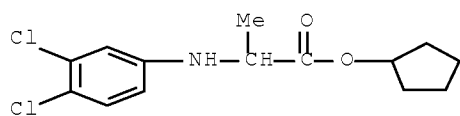
CN Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-13-3 ZCAPLUS

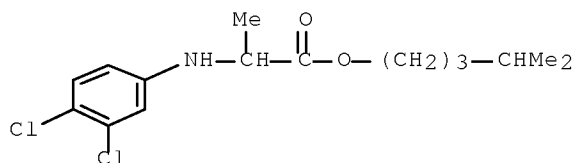
CN Alanine, N-(3,4-dichlorophenyl)-, cyclopentyl ester (CA INDEX NAME)

10/598508



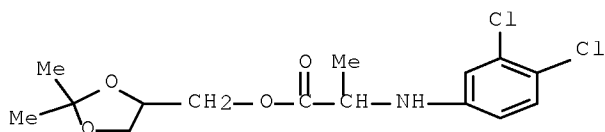
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CN Alanine, N-(3,4-dichlorophenyl)-, 4-methylpentyl ester (CA INDEX NAME)



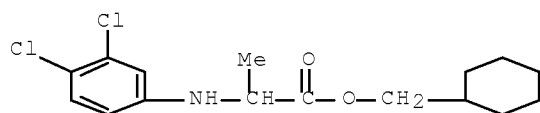
RN 208339-15-5 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, (2,2-dimethyl-1,3-dioxolan-4-yl)methyl ester (CA INDEX NAME)



RN 208339-16-6 ZCAPLUS

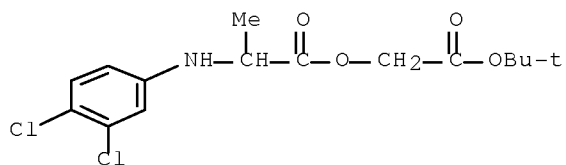
CN Alanine, N-(3,4-dichlorophenyl)-, cyclohexylmethyl ester (CA INDEX NAME)



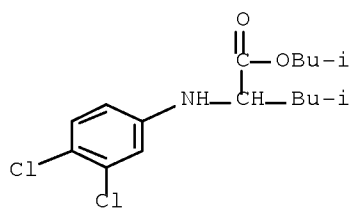
RN 208339-17-7 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-(1,1-dimethylethoxy)-2-oxoethyl ester (CA INDEX NAME)

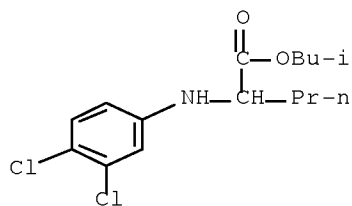
10/598508



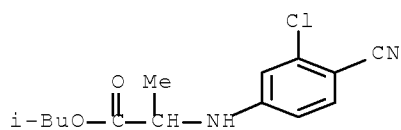
RN 208339-18-8 ZCAPLUS
CN Leucine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-19-9 ZCAPLUS
CN Norvaline, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



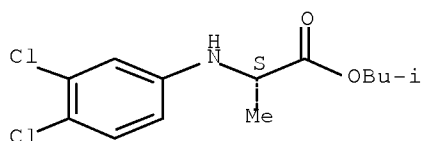
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CN Alanine, N-(3-chloro-4-cyanophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-22-4 ZCAPLUS
CN L-Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)

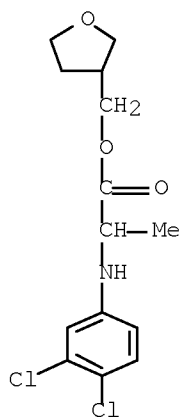
Absolute stereochemistry.

10/598508



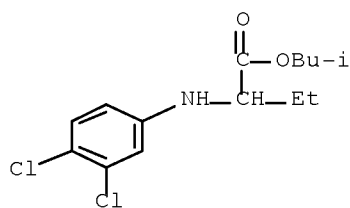
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CN Alanine, N-(3,4-dichlorophenyl)-, (tetrahydro-3-furanyl)methyl ester (CA INDEX NAME)



RN 208339-25-7 ZCAPLUS

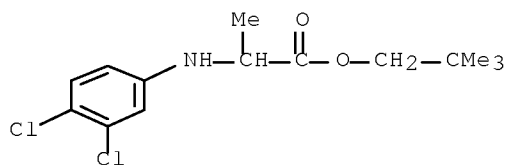
CN Butanoic acid, 2-[(3,4-dichlorophenyl)amino]-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-30-4 ZCAPLUS

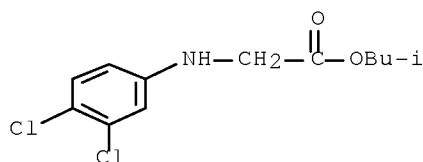
CN Alanine, N-(3,4-dichlorophenyl)-, 2,2-dimethylpropyl ester (CA INDEX NAME)

10/598508



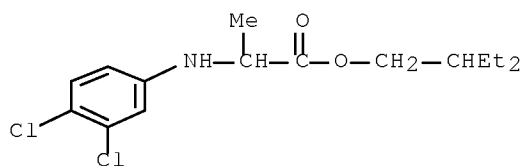
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CN Glycine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



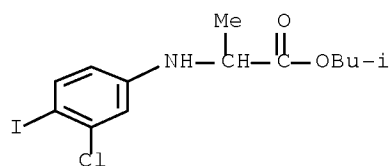
RN 208339-32-6 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-ethylbutyl ester (CA INDEX NAME)



RN 208339-33-7 ZCAPLUS

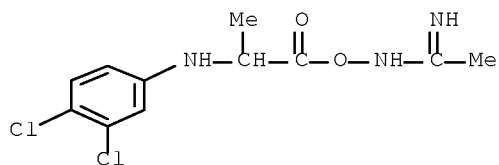
CN Alanine, N-(3-chloro-4-iodophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-38-2 ZCAPLUS

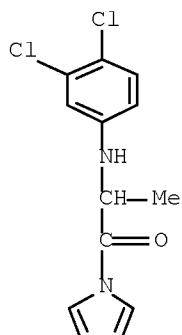
CN Ethanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)

10/598508



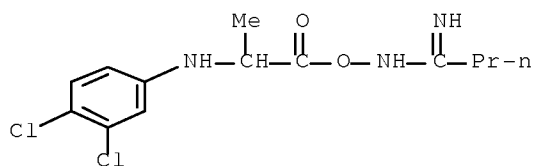
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CN 1H-Pyrrole, 1-[2-[(3,4-dichlorophenyl)amino]-1-oxopropyl]- (9CI) (CA INDEX NAME)



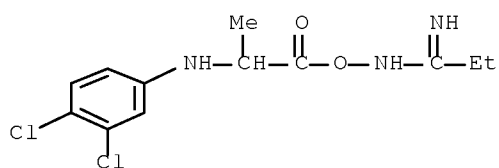
RN 208339-40-6 ZCAPLUS

CN Butanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)



RN 208339-48-4 ZCAPLUS

CN Propanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)



10/598508

IT 209983-12-0P 209983-62-0P

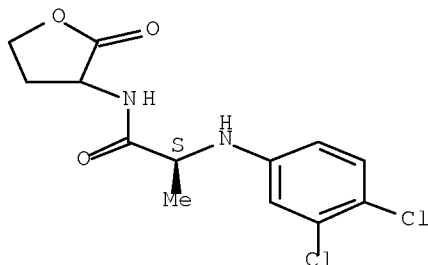
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cycloalkyl, lactam, lactone and related compds. for inhibiting β -amyloid peptide release and/or its synthesis)

RN 209983-12-0 ZCAPLUS

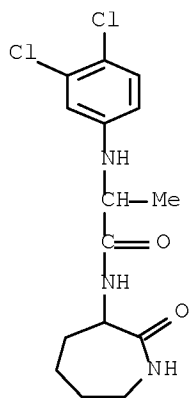
CN Propanamide, 2-[(3,4-dichlorophenyl)amino]-N-(tetrahydro-2-oxo-3-furanyl)-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 209983-62-0 ZCAPLUS

CN Propanamide, 2-[(3,4-dichlorophenyl)amino]-N-(hexahydro-2-oxo-1H-azepin-3-yl)- (CA INDEX NAME)



L58 ANSWER 44 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:352862 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:41413

TITLE: Preparation of N-aryl- and N-heteroaryl dipeptides for inhibiting β -amyloid peptide release

INVENTOR(S): Audia, James E.; Folmer, Beverly K.; John, Varghese; Latimer, Lee H.; Nissen, Jeffrey S.; Porter, Warren J.; Thorsett, Eugene D.; Wu, Jing

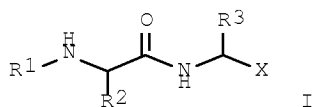
PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; Eli Lilly & Co.

10/598508

SOURCE: PCT Int. Appl., 131 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9822493	A2	19980528	WO 1997-US18704	19971120
WO 9822493	A3	19980723		
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RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2270876	A1	19980528	CA 1997-2270876	19971120
AU 9853543	A	19980610	AU 1998-53543	19971120
EP 942923	A2	19990922	EP 1997-950576	19971120
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CN 1237978	A	19991208	CN 1997-199776	19971120
BR 9714358	A	20000321	BR 1997-14358	19971120
NZ 335157	A	20010126	NZ 1997-335157	19971120
HU 2000001383	A2	20010528	HU 2000-1383	19971120
HU 2000001383	A3	20011128		
JP 2001519769	T	20011023	JP 1998-523649	19971120
US 6096782	A	20000801	US 1997-976191	19971121
US 20010020097	A1	20010906	US 1999-280966	19990330
US 6495693	B2	20021217		
MX 9904527	A	20000731	MX 1999-4527	19990514
NO 9902426	A	19990630	NO 1999-2426	19990520
PRIORITY APPLN. INFO.:			US 1996-755334	A 19961122
			US 1996-77175P	P 19961122
			WO 1997-US18704	W 19971120
			US 1997-976191	A1 19971121

OTHER SOURCE(S): MARPAT 129:41413
 GI



AB Disclosed are title compds. I [R1 = (un)substituted Ph, (un)substituted 2-naphthyl, (un)substituted heteroaryl; R2 = H, C1-4 alkyl, C1-4 alkoxy, C1-4 alkylthio, (un)substituted aryl, (un)substituted heteroaryl; R3 = (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, aryl, cycloalkyl, cycloalkenyl, heteroaryl, heterocyclyl; X = CO-Y; Y = (un)substituted alkyl, (un)substituted alkoxy, (un)substituted alkylthio, OH, aryl, heteroaryl, heterocyclyl, (un)substituted amino; with provisos] which

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inhibit β -amyloid peptide release and/or its synthesis, and, accordingly, have utility in treating Alzheimer's disease. Also disclosed are pharmaceutical compns. comprising a compound which inhibits β -amyloid peptide release and/or its synthesis as well as methods for treating Alzheimer's disease both prophylactically and therapeutically with such pharmaceutical compns. Thus, substitution of 3,4-dichloroaniline with 2-chloropropionic acid gave N-(3,4-dichlorophenyl)-DL-alanine, which underwent peptide coupling with L-valine Me ester hydrochloride to give desired title compound 3,4-Cl₂C₆H₃-DL-Ala-Val-OMe.

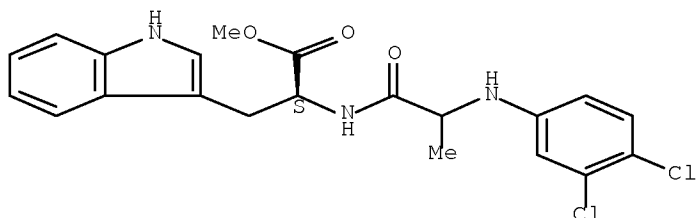
IT 208330-81-8P 208331-02-6P 208331-03-7F

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-aryl- and N-heteroaryl dipeptides for inhibiting β -amyloid peptide release)

RN 208330-81-8 ZCAPLUS

CN L-Tryptophan, N-(3,4-dichlorophenyl)alanyl-, methyl ester (9CI) (CA INDEX NAME)

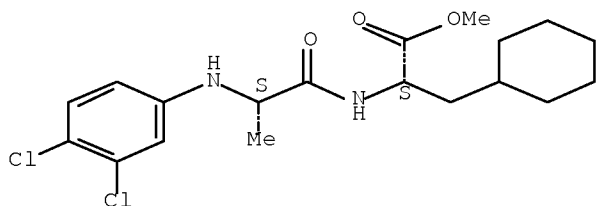
Absolute stereochemistry.



RN 208331-02-6 ZCAPLUS

CN D-Alanine, N-(3,4-dichlorophenyl)-D-alanyl-3-cyclohexyl-, methyl ester, rel- (9CI) (CA INDEX NAME)

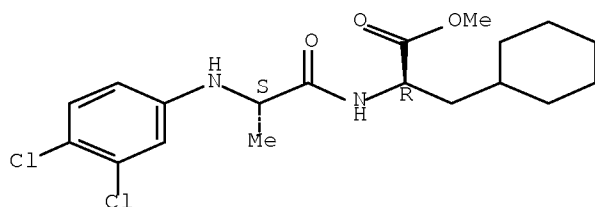
Relative stereochemistry.



RN 208331-03-7 ZCAPLUS

CN D-Alanine, N-(3,4-dichlorophenyl)-L-alanyl-3-cyclohexyl-, methyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L58 ANSWER 45 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1998:352819 ZCAPLUS Full-text
 DOCUMENT NUMBER: 129:41408
 TITLE: Preparation of N-aryl- and N-heteroaryl-amino acid esters for inhibiting β -amyloid peptide release
 INVENTOR(S): Audia, James E.; Folmer, Beverly K.; John, Varghese; Latimer, Lee H.; Nissen, Jeffrey S.; Reel, Jon K.; Thorsett, Eugene D.; Whitesitt, Celia A.
 PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; Eli Lilly & Co.
 SOURCE: PCT Int. Appl., 110 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9822441	A2	19980528	WO 1997-US20356	19971120
WO 9822441	A3	19980827		
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RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 5585198	A	19971120	AU 1998-55851	19971120
CA 2272433	A1	19980528	CA 1997-2272433	19971120
EP 944580	A2	19990929	EP 1997-952177	19971120
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JP 2001508408	T	20010626	JP 1998-523700	19971120
US 5965614	A	19991012	US 1997-975977	19971121
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PRIORITY APPLN. INFO.:				
			US 1996-104593P	P 19961122
			US 1996-755444	A 19961122
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OTHER SOURCE(S): MARPAT 129:41408				
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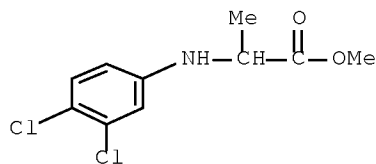
AB Disclosed are title amino acid esters I [R1 = substituted Ph group Q, (un)substituted 2-naphthyl; R2 = H, C1-4 alkyl, C1-4 alkoxy, C1-4 alkylthio; R3 = Y(CH₂)_nCHR₄R₅, ON:C(NH₂)R₆, O(CH₂)_pCO₂R₇, pyrrolo; n = 0-2; Y = O, S; R₄, R₅ = independently H, alkyl, alkenyl, optionally substituted aryl or heteroaryl; CHR₄R₅ = cycloalkyl, cycloalkenyl, or heterocyclic group; R₆ = alkyl, aryl, cycloalkyl, heteroaryl; p = 1-2, R₇ = alkyl; R₈, R₁₀ = independently H, halo, NO₂, CN, trihalomethyl, alkoxy, alkylthio; R₉ = acyl, alkyl, alkoxy, alkoxy carbonyl, alkylalkoxy, N₃, CN, halo, H, NO₂, trihalomethyl, alkylthio; R₈R₉ may form heteroaryl or heterocyclic ring containing 3-8 atoms and 1-3 heteroatoms O, N, or S; with provisos that R₈-R₁₀ are not all = H, and when R₉ = H, then both R₈ and R₁₀ ≠ H] which inhibit β-amyloid peptide release and/or its synthesis, and, accordingly, have utility in treating Alzheimer's disease. Also disclosed are pharmaceutical compns. comprising a compound which inhibits β-amyloid peptide release and/or its synthesis as well as methods for treating Alzheimer's disease both prophylactically and therapeutically with such pharmaceutical compns. Thus, reductive amination of Et pyruvate with 3,4-dichloroaniline gave 3,4-Cl₂C₆H₃-DL-Ala-OEt. Conversion of iso-Bu (R)-(+)-lactate to the corresponding triflate with trifluoromethanesulfonic anhydride, followed by substitution with 3,4-dichloroaniline gave 3,4-Cl₂C₆H₃-L-Ala-OCH₂CHMe₂.

IT 83442-68-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of N-aryl- and N-heteroarylamino acid esters for inhibiting β-amyloid peptide release)

RN 83442-68-6 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)



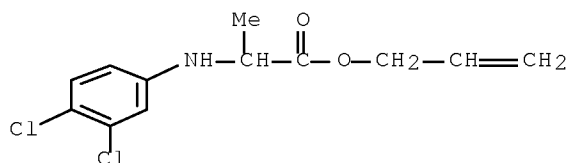
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208339-32-6P 208339-33-7P 208339-38-2P
208339-39-3P 208339-40-6P 208339-48-4P

10/598508

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-aryl- and N-heteroaryl amino acid esters for inhibiting β -amyloid peptide release)

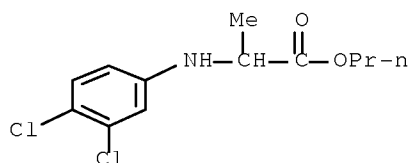
RN 83442-80-2 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-propenyl ester (9CI) (CA INDEX NAME)



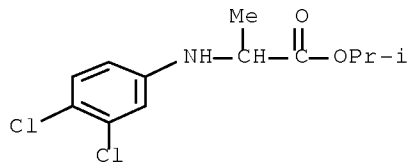
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CN Alanine, N-(3,4-dichlorophenyl)-, propyl ester (CA INDEX NAME)



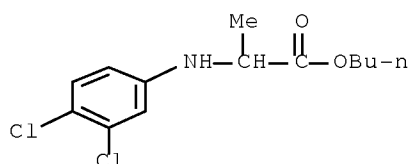
RN 106146-58-1 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 1-methylethyl ester (CA INDEX NAME)



RN 106146-59-2 ZCAPLUS

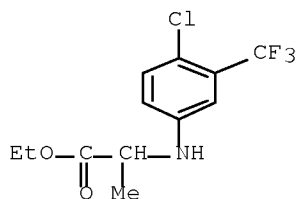
CN Alanine, N-(3,4-dichlorophenyl)-, butyl ester (CA INDEX NAME)



10/598508

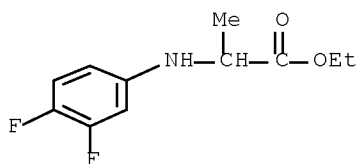
RN 208339-09-7 ZCAPLUS

CN Alanine, N-[4-chloro-3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



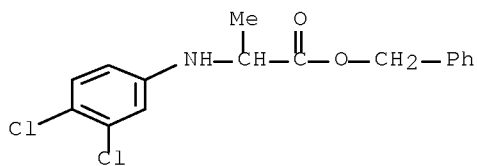
RN 208339-10-0 ZCAPLUS

CN Alanine, N-(3,4-difluorophenyl)-, ethyl ester (CA INDEX NAME)



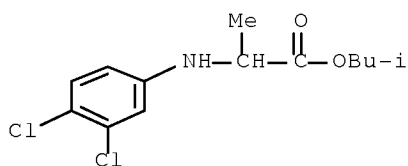
RN 208339-11-1 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, phenylmethyl ester (CA INDEX NAME)



RN 208339-12-2 ZCAPLUS

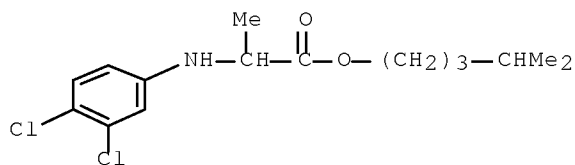
CN Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



10/598508

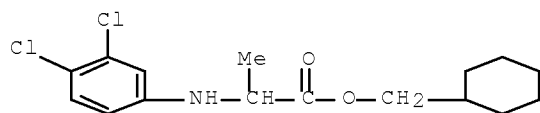
RN 208339-14-4 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 4-methylpentyl ester (CA INDEX NAME)



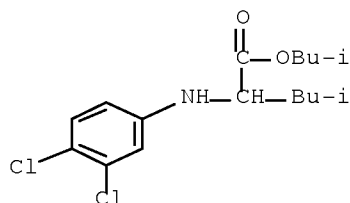
RN 208339-16-6 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, cyclohexylmethyl ester (CA INDEX NAME)



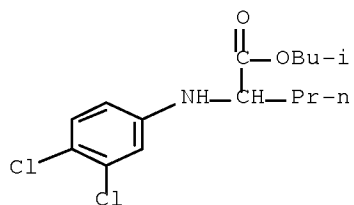
RN 208339-18-8 ZCAPLUS

CN Leucine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-19-9 ZCAPLUS

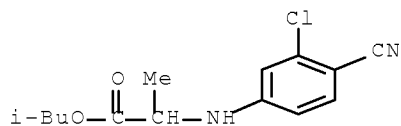
CN Norvaline, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



10/598508

RN 208339-21-3 ZCAPLUS

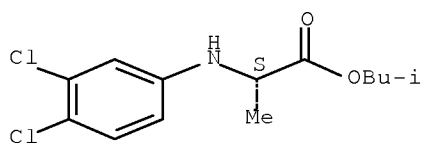
CN Alanine, N-(3-chloro-4-cyanophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-22-4 ZCAPLUS

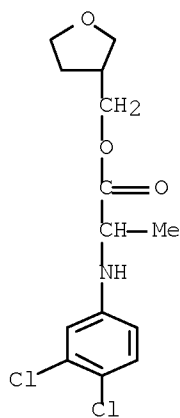
CN L-Alanine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 208339-23-5 ZCAPLUS

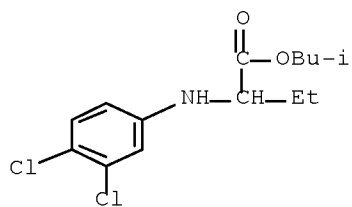
CN Alanine, N-(3,4-dichlorophenyl)-, (tetrahydro-3-furanyl)methyl ester (CA INDEX NAME)



RN 208339-25-7 ZCAPLUS

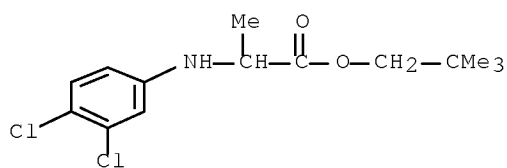
CN Butanoic acid, 2-[(3,4-dichlorophenyl)amino]-, 2-methylpropyl ester (CA INDEX NAME)

10/598508



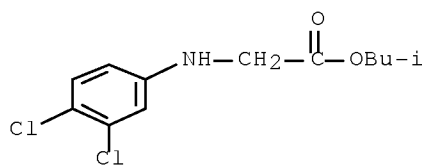
RN 208339-30-4 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2,2-dimethylpropyl ester (CA INDEX NAME)



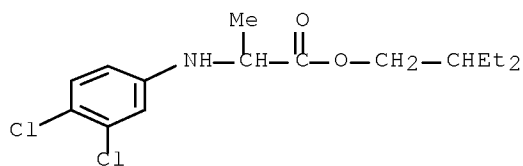
RN 208339-31-5 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)-, 2-methylpropyl ester (CA INDEX NAME)



RN 208339-32-6 ZCAPLUS

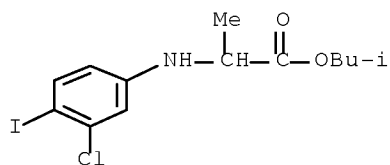
CN Alanine, N-(3,4-dichlorophenyl)-, 2-ethylbutyl ester (CA INDEX NAME)



RN 208339-33-7 ZCAPLUS

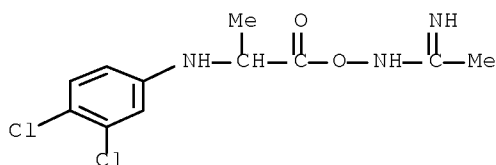
CN Alanine, N-(3-chloro-4-iodophenyl)-, 2-methylpropyl ester (CA INDEX NAME)

10/598508



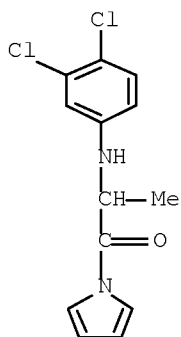
RN 208339-38-2 ZCAPLUS

CN Ethanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)



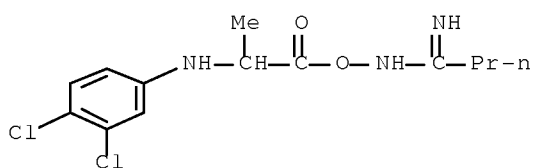
RN 208339-39-3 ZCAPLUS

CN 1H-Pyrrole, 1-[2-[(3,4-dichlorophenyl)amino]-1-oxopropyl]- (9CI) (CA INDEX NAME)



RN 208339-40-6 ZCAPLUS

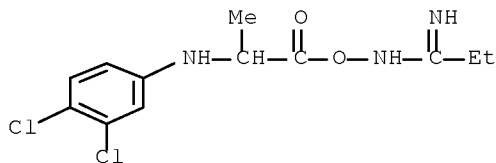
CN Butanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)



10/598508

RN 208339-48-4 ZCAPLUS

CN Propanimidamide, N-[2-[(3,4-dichlorophenyl)amino]-1-oxopropoxy]- (9CI)
(CA INDEX NAME)

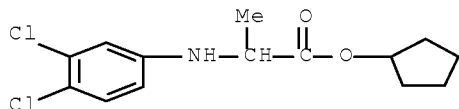


IT 208339-13-3P 208339-15-5P 208339-17-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthetic DL-alanine deriv.preparation of N-aryl- and N-heteroaryl amino acid esters for inhibiting β -amyloid peptide release)

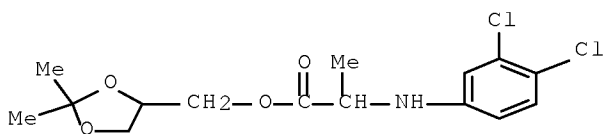
RN 208339-13-3 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, cyclopentyl ester (CA INDEX NAME)



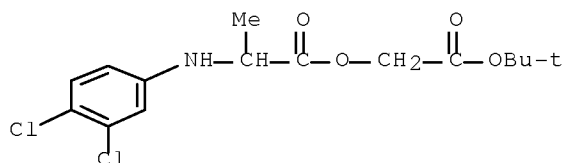
RN 208339-15-5 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, (2,2-dimethyl-1,3-dioxolan-4-yl)methyl ester (CA INDEX NAME)



RN 208339-17-7 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-(1,1-dimethylethoxy)-2-oxoethyl ester (CA INDEX NAME)



L58 ANSWER 46 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:156478 ZCAPLUS Full-text

DOCUMENT NUMBER: 120:156478

ORIGINAL REFERENCE NO.: 120:27397a,27400a

TITLE: Synthesis of Haptens and Derivation of Monoclonal Antibodies for Immunoassay of the Phenylurea Herbicide Diuron

AUTHOR(S): Karu, Alexander E.; Goodrow, Marvin H.; Schmidt, Douglas J.; Hammock, Bruce D.; Bigelow, Michael W.

CORPORATE SOURCE: College of Natural Resources Hybridoma Facility, University of California, Berkeley, CA, 94720, USA

SOURCE: Journal of Agricultural and Food Chemistry (1994), 42(2), 301-9

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A scheme is described for the synthesis of two different types of phenylurea haptens for immunization and use as detecting conjugates in enzyme immunoassays (EIAs). The haptens were used to develop indirect and direct EIAs and to derive a panel of monoclonal antibodies (MAbs) with different specificities for diuron and its analogs. One of six possible combinations of hapten-spacer arm conjugates tested as immunizing and screening antigens resulted in an indirect competition EIA that was 100-2000-fold more sensitive than the others. The eight most sensitive MAbs had I50 values of 2-20 ppb for diuron. These MAbs gave two different patterns of cross-reactivities with monuron and linuron and negligible recognition of other arylurea herbicides. These MAbs and EIAs are potentially suitable for identification as well as detection of diuron, monuron, and linuron.

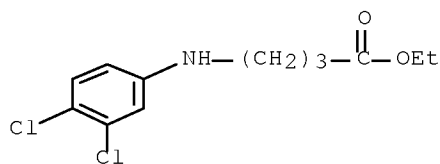
IT 83448-40-2P 153564-34-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as hapten for phenylurea herbicides, enzyme immunoassay in relation to)

RN 83448-40-2 ZCAPLUS

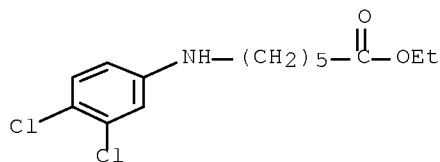
CN Butanoic acid, 4-[(3,4-dichlorophenyl)amino]-, ethyl ester (CA INDEX NAME)



RN 153564-34-2 ZCAPLUS

10/598508

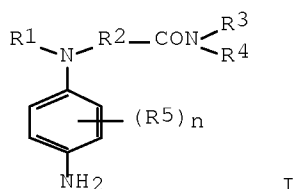
CN Hexanoic acid, 6-[(3,4-dichlorophenyl)amino]-, ethyl ester (CA INDEX NAME)



L58 ANSWER 47 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1992:500823 ZCAPLUS Full-text
 DOCUMENT NUMBER: 117:100823
 ORIGINAL REFERENCE NO.: 117:17359a,17362a
 TITLE: Color photographic image formation
 INVENTOR(S): Yamamoto, Soichiro; Oki, Nobutaka; Taniguchi, Masato
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 43 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03245142	A	19911031	JP 1990-40941	19900223
PRIORITY APPLN. INFO.:			JP 1990-40941	19900223
OTHER SOURCE(S):	MARPAT 117:100823			

GI

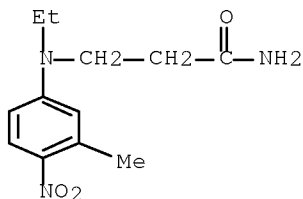


AB A method for processing a Ag halide color photog. material having ≥ 1 halide emulsion layer(s) containing Ag chloride ≥ 90 mol% involves utilizing a developer solution containing I (R1 = alkyl; R2 = alkylene; R3,4 = H, C \leq 4 alkyl; R5 = alkyl, halo, group bonded via N or O; n = 0-4), and bleaching for 5-20 s. A rapid and stable processing is achieved.

IT 142155-78-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, photog. developer from)

RN 142155-78-0 ZCAPLUS

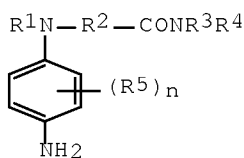
CN Propanamide, 3-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 48 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1992:479838 ZCAPLUS Full-text
 DOCUMENT NUMBER: 117:79838
 ORIGINAL REFERENCE NO.: 117:13787a,13790a
 TITLE: Method for color imaging
 INVENTOR(S): Taniguchi, Masato; Oki, Nobutaka; Nakamura, Koichi
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 57 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 03246542	A	19911101	JP 1990-43793	19900223
PRIORITY APPLN. INFO.:			JP 1990-43793	19900223

GI



I

AB A method for color imaging involves development of a Ag halide color photog. material containing at least one acetanilide yellow coupler R11COCHR12X11 (R11 = C4-20 tert-alkyl; R12 = CONHPh; X11 = group leaving upon reaction with the oxidized form of a developing agent) by using a processing solution containing at least one developing agent (I; R1 = alkyl; R2 = C≥2 alkylene; R3, R4 = H, C≤4 alkyl; R5 = alkyl, halo, substituent linked though N or O; n = 0-4; when n ≥2, R5 is same or different). The imaging method improves light-stability of yellow dyes.

IT 142155-78-0P

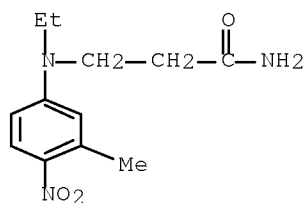
RL: PREP (Preparation)

(preparation of, as intermediate for yellow photog. coupler)

RN 142155-78-0 ZCAPLUS

CN Propanamide, 3-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)

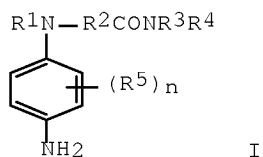
10/598508



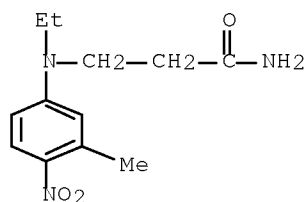
L58 ANSWER 49 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1992:436467 ZCAPLUS Full-text
 DOCUMENT NUMBER: 117:36467
 ORIGINAL REFERENCE NO.: 117:6341a,6344a
 TITLE: Color photographic developing agents, processing compositions containing them, and color imaging method using the compositions
 INVENTOR(S): Taniguchi, Masato; Oki, Nobutaka; Nakamura, Koichi
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 56 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03246543	A	19911101	JP 1990-43792	19900223
JP 2631147	B2	19970716		
PRIORITY APPLN. INFO.:			JP 1990-43792	19900223
OTHER SOURCE(S):	MARPAT 117:36467			

GI

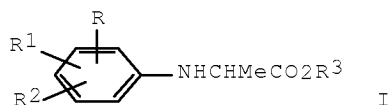


AB Color photog. developing agents (I; R1 = alkyl; when R2 = C_≥2 alkylene, R3 = H, C_≤4 alkyl and R4 = H; when R2 = C_≥3 alkylene, R3, R4 = H, C_≤4 alkyl; R6 = substituent; n = 0-4; when n _≥2, R6 is same or different) are prepared
 Processing compns. for Ag halide color photog. materials contain at least one I. A color imaging method involves development of Ag halide color photog. materials by processing compns. containing at least one I.
 IT 142155-78-0F
 RL: PREP (Preparation)
 (preparation of, as intermediate for preparing color photog. developing agent)
 RN 142155-78-0 ZCAPLUS
 CN Propanamide, 3-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 50 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1992:189639 ZCAPLUS Full-text
 DOCUMENT NUMBER: 116:189639
 ORIGINAL REFERENCE NO.: 116:31991a,31994a
 TITLE: Synergistic insecticidal compositions comprising phenylalanine esters
 INVENTOR(S): Weber, Bernd; Otto, Dieter; Lyr, Horst; Strumpf, Thomas; Karabensch, Karl Heinz; Kempster, Peter; Damm, Heinz
 PATENT ASSIGNEE(S): Biologische Zentralanstalt Berlin, Germany
 SOURCE: Ger. (East), 9 pp.
 CODEN: GEXXA8
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 295524	A5	19911107	DD 1986-297283	19861209
PRIORITY APPLN. INFO.:			DD 1986-297283	19861209
OTHER SOURCE(S):	MARPAT	116:189639		
GI				



AB Synergistic compns. comprise a phenylalanine derivative ester I (R, R1, R2 = H, C1-4 alkyl, halo, C1-4 alkoxy; R3 = C1-12 alkyl, C2-4 haloalkyl, C3-6 alkenyl, etc.) and a known organophosphorus insecticide (Markush given). A mixture of I (R = R1 = R2 = H, R3 = hexyl) and trichlorophon had a synergistic contact insecticidal activity against *Sitophilus granarius*.
 IT 139641-08-0 139641-35-3 139641-59-1
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
 (insecticide, synergistic)
 RN 139641-08-0 ZCAPLUS

10/598508

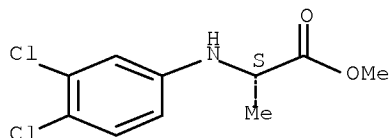
CN L-Alanine, N-(3,4-dichlorophenyl)-, methyl ester, mixt. with dimethyl
(2,2,2-trichloro-1-hydroxyethyl)phosphonate (9CI) (CA INDEX NAME)

CM 1

CRN 139641-07-9

CMF C10 H11 Cl2 N O2

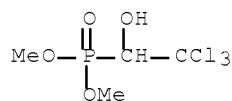
Absolute stereochemistry.



CM 2

CRN 52-68-6

CMF C4 H8 Cl3 O4 P



RN 139641-35-3 ZCAPLUS

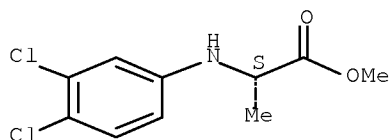
CN L-Alanine, N-(3,4-dichlorophenyl)-, methyl ester, mixt. with
1,2-dibromo-2,2-dichloroethyl dimethyl phosphate (9CI) (CA INDEX NAME)

CM 1

CRN 139641-07-9

CMF C10 H11 Cl2 N O2

Absolute stereochemistry.

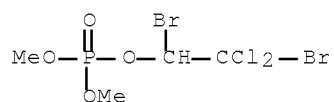


CM 2

CRN 300-76-5

CMF C4 H7 Br2 Cl2 O4 P

10/598508

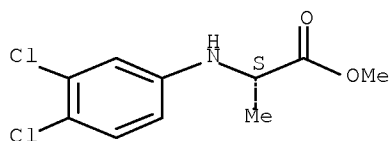


RN 139641-59-1 ZCAPLUS
CN L-Alanine, N-(3,4-dichlorophenyl)-, methyl ester, mixt. with
2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl phosphate (9CI) (CA INDEX
NAME)

CM 1

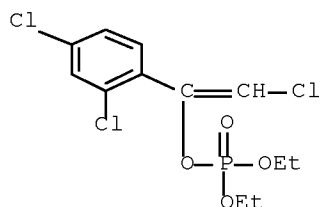
CRN 139641-07-9
CMF C10 H11 Cl2 N O2

Absolute stereochemistry.



CM 2

CRN 470-90-6
CMF C12 H14 Cl3 O4 P



L58 ANSWER 51 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:146185 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 116:146185
ORIGINAL REFERENCE NO.: 116:24581a,24584a
TITLE: Synergistic insecticidal compositions comprising a
phenylalanine ester and a carbamate
INVENTOR(S): Weber, Bernd; Strumpf, Thomas; Otto, Dieter; Lyr,
Horst; Karabensch, Karl Heinz
PATENT ASSIGNEE(S): Biologische Zentralanstalt Berlin, Germany

10/598508

SOURCE: Ger. (East), 7 pp.
 CODEN: GEXXA8
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 295523	A5	19911107	DD 1986-297288	19861209
PRIORITY APPLN. INFO.:			DD 1986-297288	19861209
OTHER SOURCE(S):	MARPAT	116:146185		

GI



AB The title compns. comprise a phenylalanine ester [I; R,R1,R2 = H, alkyl, alkoxy, halo; R3 = alkyl, cycloalkyl, alkoxyalkyl, diaminoalkyl, (un)substituted Ph, benzyl or phenylethyl] and a known carbamate insecticide. A mixture of carbofuran and I (R = 2-Me, R1 = R2 = H, R3 = Me) synergistically controlled the housefly.

IT 139641-95-5
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
 (insecticide, synergistic)

RN 139641-95-5 ZCAPLUS

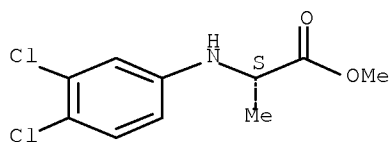
CN L-Alanine, N-(3,4-dichlorophenyl)-, methyl ester, mixt. with 2,3-dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate (9CI) (CA INDEX NAME)

CM 1

CRN 139641-07-9

CMF C10 H11 C12 N O2

Absolute stereochemistry.

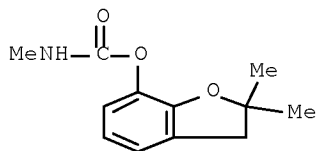


CM 2

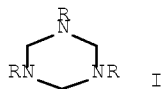
CRN 1563-66-2

10/598508

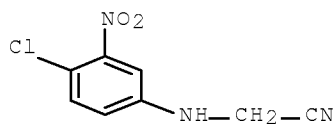
CMF C12 H15 N O3



L58 ANSWER 52 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:448830 ZCAPLUS Full-text
DOCUMENT NUMBER: 115:48830
ORIGINAL REFERENCE NO.: 115:8465a,8468a
TITLE: Titanium tetrachloride induced N-methyleneamine
equivalents: a new route to aminoacetonitriles
AUTHOR(S): Ha, Hyun Joon; Nam, Gong Sil; Park, Kyong Pae
CORPORATE SOURCE: Div. Chem., Korea Inst. Sci. Technol., Seoul, 130-650,
S. Korea
SOURCE: Synthetic Communications (1991), 21(2), 155-60
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:48830
GI



AB TiCl4-induced N-methyleneamine equivalent from hexahydro-1,3,5-triazines I (R
= alkyl, cyclohexyl, Ph, p-O2NC6H4, PhCH2) or N-(methoxymethyl)amines
RNHCH2OMe (R = substituted phenyl) were treated with Me3SiCN cyanide to give
aminoacetonitriles RNHCH2CN in 40-90% yield.
IT 117887-53-3F
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 117887-53-3 ZCAPLUS
CN Acetonitrile, [(4-chloro-3-nitrophenyl)amino]- (9CI) (CA INDEX NAME)

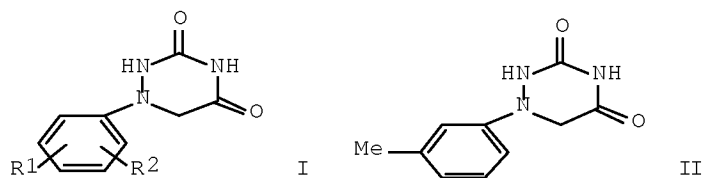


L58 ANSWER 53 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

10/598508

ACCESSION NUMBER: 1991:81891 ZCAPLUS Full-text
DOCUMENT NUMBER: 114:81891
ORIGINAL REFERENCE NO.: 114:13989a,13992a
TITLE: Preparation of 1-phenyl-1,2,4-triazine-3,5-(2H,4H)diones as 5-lipoxygenase inhibitors
INVENTOR(S): Ellis, Frank; Naylor, Alan; Wallis, Christopher John; Waterhouse, Ian
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Eur. Pat. Appl., 47 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 388165	A2	19900919	EP 1990-302694	19900314
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 2012004	A1	19900915	CA 1990-2012004	19900313
NO 9001201	A	19900917	NO 1990-1201	19900314
HU 54125	A2	19910128	HU 1990-1569	19900314
US 5023255	A	19910611	US 1990-493250	19900314
AU 9051369	A	19900920	AU 1990-51369	19900315
JP 02289555	A	19901129	JP 1990-62866	19900315
ZA 9001990	A	19910327	ZA 1990-1990	19900315
PRIORITY APPLN. INFO.:			GB 1989-5914	A 19890315
			GB 1989-24135	A 19891026
			GB 1989-24138	A 19891026
OTHER SOURCE(S):	MARPAT 114:81891			
GI				

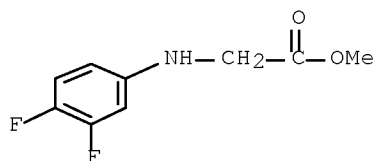


AB The title compds. [I; R1 = halo, alkyl, alkoxy, alkoxyalkoxy, (substituted) PhO, phenylalkoxy; R2 = H, halo, OH, alkyl, alkoxy], were prepared as 5-lipoxygenase inhibitors (no data). Thus, Me [1-(3-methylphenyl)hydrazino]acetate (preparation for m-toluidine and ClCH2CO2Me given) and NaOCN in PhMe were treated dropwise with F3CCO2H in PhMe to give a urea which in MeOH was added to NaOMe in MeOH to give title compound II.

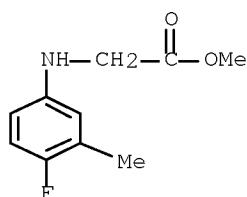
IT 126689-85-8P 131770-62-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for phenyltriazinedione lipoxygenase inhibitor)

RN 126689-85-8 ZCAPLUS
CN Glycine, N-(3,4-difluorophenyl)-, methyl ester (CA INDEX NAME)

10/598508

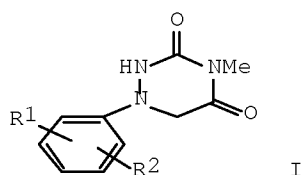


RN 131770-62-2 ZCAPLUS
CN Glycine, N-(4-fluoro-3-methylphenyl)-, methyl ester (CA INDEX NAME)



L58 ANSWER 54 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:198426 ZCAPLUS Full-text
DOCUMENT NUMBER: 112:198426
ORIGINAL REFERENCE NO.: 112:33557a,33560a
TITLE: Preparation and formulation of dihydro-4-methyl-1-phenyl-1,2,4-triazine-3,5-(2H,4H)-diones as 5-lipoxygenase inhibitors
INVENTOR(S): Waterhouse, Ian; Naylor, Alan; Wallis, Christopher John; Ellis, Frank
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Eur. Pat. Appl., 22 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
EP 340030	A2	19891102	EP 1989-304308	19890428
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 8902070	A	19891030	DK 1989-2070	19890428
FI 8902041	A	19891030	FI 1989-2041	19890428
AU 8933771	A	19891102	AU 1989-33771	19890428
JP 02011557	A	19900116	JP 1989-107883	19890428
ZA 8903193	A	19900425	ZA 1989-3193	19890428
US 4985427	A	19910115	US 1989-344667	19890428
PRIORITY APPLN. INFO.:			GB 1988-10185	A 19880429
OTHER SOURCE(S):	MARPAT 112:198426			
GI				



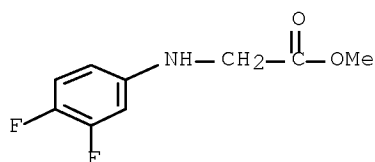
AB Title compds. I [R1 = H, halo, HO, C1-6 alkyl, C1-6 alkoxy, (un)substituted phenyl-C1-3-alkoxy, R3O2C (R3 = H, C1-4 alkyl), R5R4NCO (R4, R5 = H, C1-4 alkyl, or R5R4N = saturated 5-7-membered heterocyclyl; R2 = H, halo, HO, C1-6 alkyl, C1-6 alkoxy] and salts thereof, for use in treatment of diseases in which leukotrienes or other 5-lipoxygenase products are mediators (no data), were prepared Me [1-(3-bromophenyl)hydrazino]acetate (preparation given) and MeNCO in MeCN was refluxed for 2 h to give I (R1 = H, R2 = 3-Br). Three pharmaceuticals containing I, 26 syntheses of I, and 46 intermediate preps. are described.

IT 126689-85-8F

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for phenyltriazinedione lipoxygenase inhibitors)

RN 126689-85-8 ZCAPLUS

CN Glycine, N-(3,4-difluorophenyl)-, methyl ester (CA INDEX NAME)



L58 ANSWER 55 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:99249 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 112:99249

ORIGINAL REFERENCE NO.: 112:16899a,16902a

TITLE: Preparation of optically active N-phenylalanine herbicides

INVENTOR(S): Miedema, Alle

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.,
Neth.

SOURCE: Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

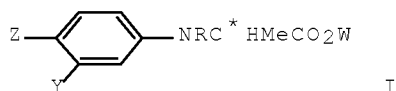
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 333282	A1	19890920	EP 1989-200631	19890310
EP 333282	B1	19930609		

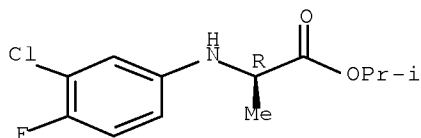
10/598508

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
 AT 90334 T 19930615 AT 1989-200631 19890310
 ES 2055005 T3 19940816 ES 1989-200631 19890310
 HU 49845 A2 19891128 HU 1989-1221 19890314
 HU 200994 B 19900928
 JP 02004747 A 19900109 JP 1989-59874 19890314
 PRIORITY APPLN. INFO.: GB 1988-6223 A 19880316
 EP 1989-200631 A 19890310
 OTHER SOURCE(S): MARPAT 112:99249
 GI



AB Optically active title compds. I [Y, Z = H, Cl, F; W = H, (halo)alkyl, alkenyl, cycloalkyl, aryl, aralkyl, alkaryl, N:CR₁R₂; R₁, R₂ = H, alkyl, aryl, aralkyl, alkaryl; R₁R₂ = alkylene may interrupted by ≥1 heteroatoms; R = PhCO], useful as herbicides (no data), are prepared by benzylation of I (R = H; the C with an asterisk has R-configuration) with a benzylation agent in the presence of a solvent and a tertiary amine. To a PhMe solution of (R)-(+)-I (R = H, Y = Cl, Z = F, W = Me₂CH) (84.6% optical purity) and Et₃N was added PhCOCl to give (R)-(-)-I (R = PhCO, Y = Cl, Z = F, W = Me₂CH) (II) (74.0% optical purity), vs 53% optical purity II from the starting material having 85.5% optical purity without Et₃N.
 IT 62836-63-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (benzylation of, in preparation of herbicide)
 RN 62836-63-9 ZCAPLUS
 CN D-Alanine, N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 56 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1989:614195 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 111:214195
 ORIGINAL REFERENCE NO.: 111:35517a,35520a
 TITLE: Synthesis of chloroacetamide compounds and their herbicidal activities
 AUTHOR(S): Hong, Moo Ki; Jeong, Young Ho; Oh, Se Mun
 CORPORATE SOURCE: Agric. Chem. Res. Inst., Rural Dev. Adm., Suwon, S. Korea
 SOURCE: Han'guk Nonghwa Hakhoechi (1988), 31(3), 234-40

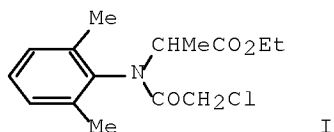
DOCUMENT TYPE:

Journal

LANGUAGE:

Korean

GI



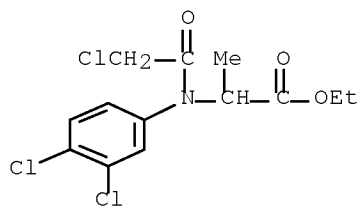
AB Some chloroacetamide derivs. were synthesized from 2,6-dialkylaniline, 4-chloroaniline, or 3,4-dichloroaniline with alkyl 2-bromopropionate and chloroacetyl chloride. It was found that N-(1'-ethoxycarbonyl-2'-chloroacetyl)-N-(2,6-dimethylphenyl)alanine (I) has the highest herbicidal effect on grass weeds. Whereas, some chloroacetamide derivs. derived from 4-chloroaniline or 3,4-dichloroaniline had very weak herbicidal effects on grass and broad leaf weeds.

IT 123695-98-7P 123695-99-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and herbicidal activity of)

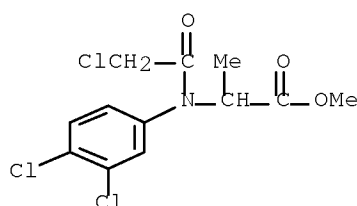
RN 123695-98-7 ZCAPLUS

CN Alanine, N-(chloroacetyl)-N-(3,4-dichlorophenyl)-, ethyl ester (9CI) (CA INDEX NAME)

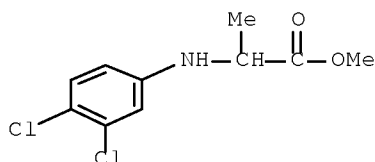


RN 123695-99-8 ZCAPLUS

CN Alanine, N-(chloroacetyl)-N-(3,4-dichlorophenyl)-, methyl ester (9CI) (CA INDEX NAME)



IT 83442-68-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and N-chloroacetylation of)
 RN 83442-68-6 ZCAPLUS
 CN Alanine, N-(3,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)



L58 ANSWER 57 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1988:204508 ZCAPLUS Full-text
 DOCUMENT NUMBER: 108:204508
 ORIGINAL REFERENCE NO.: 108:33601a,33604a
 TITLE: Preparation of dihydroquinolinone-4-oximes as
 diuretics
 INVENTOR(S): Mochida, Ei; Uemura, Akio; Kato, Kazuo; Tokunaga,
 Hiroki; Haga, Akinori
 PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan; Hodogaya
 Chemical Co., Ltd.
 SOURCE: Eur. Pat. Appl., 91 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 243982	A1	19871104	EP 1987-106373	19870430
EP 243982	B1	19910417		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 63239270	A	19881005	JP 1987-92788	19870415
JP 04046951	B	19920731		
US 4839368	A	19890613	US 1987-42784	19870427
ZA 8703133	A	19871230	ZA 1987-3133	19870430
AT 62679	T	19910515	AT 1987-106373	19870430
ES 2036542	T3	19930601	ES 1987-106373	19870430
AU 8772441	A	19871105	AU 1987-72441	19870501
AU 596657	B2	19900510		
WO 8706580	A1	19871105	WO 1987-JP276	19870501
W: DK, FI, HU, KR, LK, NO, SU				
HU 47912	A2	19890428	HU 1987-2931	19870501
HU 199803	B	19900328		
IL 82399	A	19920621	IL 1987-82399	19870501
IL 97150	A	19920621	IL 1987-97150	19870501
CA 1314888	C	19930323	CA 1987-536174	19870501

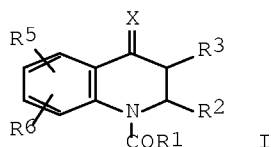
10/598508

FI 8705771	A	19871230	FI 1987-5771	19871230
FI 90071	B	19930915		
FI 90071	C	19931227		
NO 8705495	A	19880301	NO 1987-5495	19871230
NO 174465	B	19940131		
NO 174465	C	19940511		
DK 8706944	A	19880302	DK 1987-6944	19871230
DK 171379	B1	19961007		
SU 1722227	A3	19920323	SU 1987-4203894	19871230
SU 1779246	A3	19921130	SU 1988-4613166	19881223
US 5077410	A	19911231	US 1989-301125	19890125
AU 9058618	A	19901115	AU 1990-58618	19900702
AU 630716	B2	19921105		
JP 05262737	A	19931012	JP 1992-27135	19920118
JP 08000812	B	19960110		
CA 1333286	C	19941129	CA 1992-616521	19921130

PRIORITY APPLN. INFO.:

JP 1986-102847	A	19860502
JP 1987-92788	A	19870415
US 1987-42784	A3	19870427
EP 1987-106373	A	19870430
CA 1987-536174	A3	19870501
IL 1987-82399	A	19870501
WO 1987-JP276	W	19870501

OTHER SOURCE(S): CASREACT 108:204508; MARPAT 108:204508
GI



AB The title compds. [I; R1 = alkyl, haloalkyl, cycloalkyl, alkoxy, MeOCH2, MeO2CCH2CH2, PhCH2, PhCH:CH, naphthyl, pyridyl, thienyl, pyrazinyl, (un)substituted Ph; R2, R3 = H, Me; R5, R6 = H, halo, OH, MeS, MeS(O), MeSO2, NMe2, NO2, Ac, Me, CF3, CO2Me, MeO; X = NOR4; R4 = CH2CO2Me, SO3H, MeSO2, P(O)(OMe)OH] were prepared 2,4-Cl2C6H3COCl was added to 7-chloro-2,3-dihydro-4-1H-quinolinone in dioxane containing pyridine and the mixture stirred 3 h to give I (R1 = 2,4-Cl2C6H3, R2 = R3 = R5 = R6 = H, X = O) to which, in MeOH, was added H2NOSO3H to give, on workup, I (R1 = 2,4-Cl2C6H3, R2 = R3 = R5 = R6 = H, X = NOSO3K) (II) which, at 0.1 mg/kg i.v., increased urine output of anesthetized dogs by 518%. II 100, lactose 890, and Mg stearate 10 g were mixed to give a 10% powder.

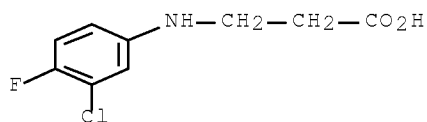
IT 114417-22-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of diuretics)

RN 114417-22-0 ZCAPLUS

CN β -Alanine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)

10/598508



L58 ANSWER 58 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:407428 ZCAPLUS Full-text

DOCUMENT NUMBER: 107:7428

ORIGINAL REFERENCE NO.: 107:1375a,1378a

TITLE: Benzo[i,j]quinolizine-2-carboxylic acid derivatives, their salts, hydrates, and pharmaceutical compositions

INVENTOR(S): Takagi, Atsushi; Kikuchi, Toshiaki; Yajima, Masao; Saeki, Masaki

PATENT ASSIGNEE(S): Tokyo Tanabe Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 61 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

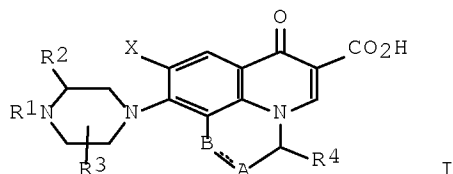
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 203795	A2	19861203	EP 1986-303948	19860523
EP 203795	A3	19880210		
EP 203795	B1	19920729		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AU 8657484	A	19861127	AU 1986-57484	19860515
AU 585981	B2	19890629		
CA 1253154	A1	19890425	CA 1986-509221	19860515
US 4720495	A	19880119	US 1986-865530	19860520
JP 62053987	A	19870309	JP 1986-117466	19860523
JP 03007674	B	19910204		
AT 78822	T	19920815	AT 1986-303948	19860523
PRIORITY APPLN. INFO.:			JP 1985-110226	A 19850524
			JP 1985-110227	A 19850524
			EP 1986-303948	A 19860523

OTHER SOURCE(S): CASREACT 107:7428; MARPAT 107:7428
GI



AB Title compds. I (R1 = H, C1-3 alkyl, HOCH2CH2; R2, R3 = H, Me, Et, R3 may be attached to same C as R2; R4 = Me, Et; X = halo; A = H2C and B = CO when A and B form a single bond or AB = CH:CH) and their salts, useful as antibacterials,

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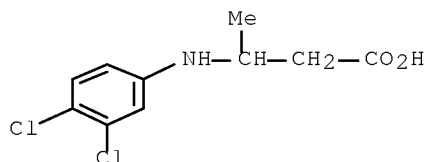
were prepared Et 9-fluoro-5-methyl-8-(4-methyl-1- piperazinyl)-6,7-dihydro-1,7-dioxo-1H,5H-benzo[i,j]quinolizine-2- carboxylate prepared in 5 steps was saponified to give I (R1 = Me, R2, R3 = H; R4 = Me; X = F; A = CH2; B = CO) (II). II showed an ED50 of 0.52 mg/kg in mice infected with Escherichia coli.

IT 34129-52-7F 108404-95-1F

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclocondensation of)

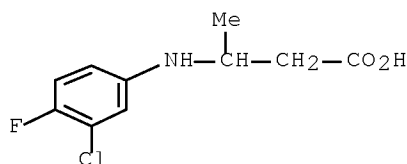
RN 34129-52-7 ZCAPLUS

CN Butanoic acid, 3-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



RN 108404-95-1 ZCAPLUS

CN Butanoic acid, 3-[(3-chloro-4-fluorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 59 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:28836 ZCAPLUS Full-text

DOCUMENT NUMBER: 106:28836

ORIGINAL REFERENCE NO.: 106:4779a,4782a

TITLE: Plant growth regulators

INVENTOR(S): Kamuro, Yasuo; Hirai, Yasuichi; Yamamoto, Susumu; Suzuki, Fumio; Shindo, Noboru

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

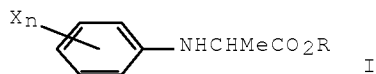
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 61152604	A	19860711	JP 1984-279527	19841226
PRIORITY APPLN. INFO.:			JP 1984-279527	19841226
OTHER SOURCE(S):	CASREACT 106:28836			

GI



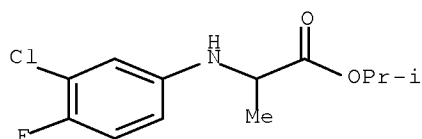
AB The alanine derivs. I (X = halo, CF₃; R = H, alkyl, alkenyl, metal, etc.; n = 0-2) are prepared as plant growth regulators. Thus, 14.6 g 3-chloro-4-fluoroaniline was reacted with 12.1 g Et α- bromopropionate in MeCN to give 10.0 g N-(3-chloro-4-fluorophenyl)alanine Et ester (II). II, applied at 2000 ppm, totally controlled citrus germination.

IT 52756-24-8P 83442-76-6P 83442-80-2P
106146-54-7P 106146-55-8P 106146-56-9P
106146-57-0P 106146-58-1P 106146-59-2P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as plant growth regulator)

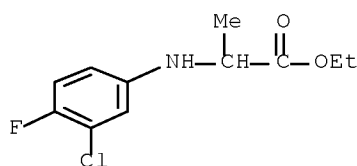
RN 52756-24-8 ZCAPLUS

CN Alanine, N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester (CA INDEX NAME)



RN 83442-76-6 ZCAPLUS

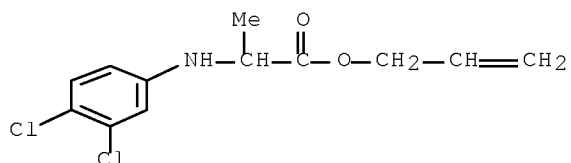
CN Alanine, N-(3-chloro-4-fluorophenyl)-, ethyl ester (CA INDEX NAME)



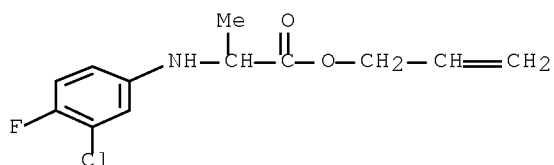
RN 83442-80-2 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-propenyl ester (9CI) (CA INDEX NAME)

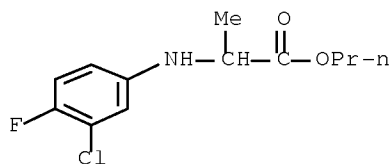
10/598508



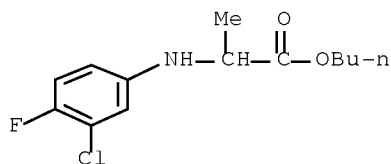
RN 106146-54-7 ZCAPLUS
CN Alanine, N-(3-chloro-4-fluorophenyl)-, 2-propenyl ester (9CI) (CA INDEX NAME)



RN 106146-55-8 ZCAPLUS
CN Alanine, N-(3-chloro-4-fluorophenyl)-, propyl ester (CA INDEX NAME)

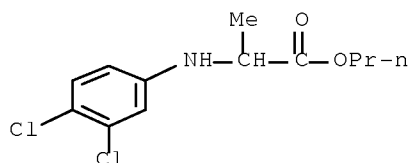


RN 106146-56-9 ZCAPLUS
CN Alanine, N-(3-chloro-4-fluorophenyl)-, butyl ester (CA INDEX NAME)



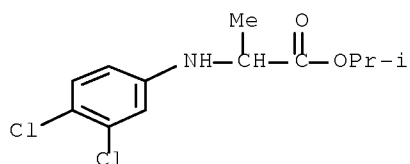
RN 106146-57-0 ZCAPLUS
CN Alanine, N-(3,4-dichlorophenyl)-, propyl ester (CA INDEX NAME)

10/598508



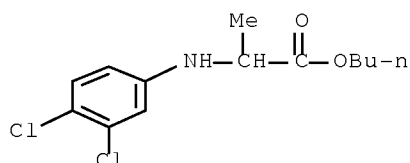
RN 106146-58-1 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 1-methylethyl ester (CA INDEX NAME)



RN 106146-59-2 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, butyl ester (CA INDEX NAME)



L58 ANSWER 60 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:19003 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 106:19003

ORIGINAL REFERENCE NO.: 106:3273a,3276a

TITLE: Amino acids. 4. Enantioselective synthesis of
N-substituted α -amino carboxylic acids from
 α -hydroxy carboxylic acids

AUTHOR(S): Effenberger, Franz; Burkard, Ulrike; Willfahrt,
Joachim

CORPORATE SOURCE: Inst. Org. Chem., Univ. Stuttgart, Stuttgart,
D-7000/80, Fed. Rep. Ger.

SOURCE: Liebigs Annalen der Chemie (1986), (2), 314-33
CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 106:19003

AB The SN2 substitution reaction of α -hydroxy carboxylic acid O-triflate (S)-
CF₃SO₃CHRCO₂R₁ (I; R = Me, R₁ = Et) with amines R₂R₃NH (R₂ = H, R₃ = hexyl,
Me₃C, PhCH₂, Ph, etc.; R₂ = Me, R₃ = PhCH₂, Ph; R₂ = R₃ = Et) gave (R)-

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alanines (R)-R₂R₃NCHMeCO₂Et. I (R = Me, CH₂Ph, R₁ = Me; R = CH₂CO₂Et, R₁ = Et) also underwent S_N2 substitution with amines to give the corresponding (R)-amino acids. The rates of substitution for (S)-MeCHR₄CO₂Et decrease for R₄ in the following order: CF₃SO₃ >> Br > MeSO₃, ≥ p-MeC₆H₄SO₃ > Cl. In the reactions with amines, decreasing reactivity affords increasing racemization and elimination as a result of the more drastic conditions.

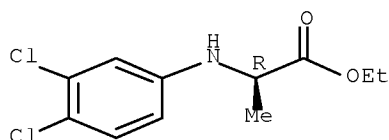
IT 62840-19-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 62840-19-1 ZCAPLUS

CN D-Alanine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 61 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:608832 ZCAPLUS Full-text

DOCUMENT NUMBER: 105:208832

ORIGINAL REFERENCE NO.: 105:33675a,33678a

TITLE: Folate antagonists. Part 23. Synthesis of selected 3-substituted-pyrimido[5,4-e]-1,2,4-triazine-5,7-diamines as potential folate antagonists

AUTHOR(S): Werbel, Leslie M.; Elslager, Edward F.; Johnson, Judith L.

CORPORATE SOURCE: Pharm. Res., Warner-Lambert/Parke-Davis, Ann Arbor, MI, 48105, USA

SOURCE: Journal of Heterocyclic Chemistry (1985), 22(5), 1369-72

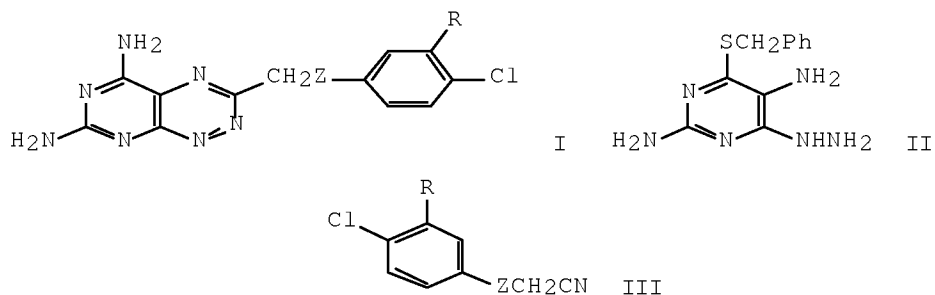
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 105:208832

GI



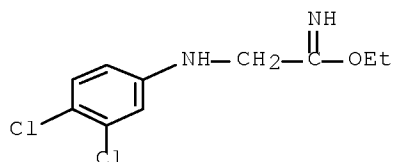
10/598508

AB Pyrimido[5,4-e]-1,2,4-triazine-5,7-diamines I (Z = NH, R = Cl; Z = S, R = H) were prepared by ring closure of hydrazino-2,5-pyrimidinediamine II with III. These nonclassical analogs of known dihydrofolate reductase inhibitors were inactive against malarial infections in mice and L1210 leukemia in vitro.

IT 104856-91-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclocondensation of, with
 hydrazino(phenylthio)pyrimidined
 iamine, pyrimidotriazine from)

RN 104856-91-9 ZCAPLUS

CN Ethanimidic acid, 2-[(3,4-dichlorophenyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



L58 ANSWER 62 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:497894 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 105:97894

ORIGINAL REFERENCE NO.: 105:15845a,15848a

TITLE: Thermal stability of N-aryl-substituted α -amino acids

AUTHOR(S): Antipanova, V. E.; Gil'mkhanova, V. T.; Maslennikova, V. V.

CORPORATE SOURCE: USSR

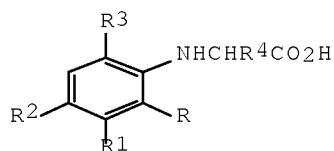
SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1986), 59(1), 222-4
 CODEN: ZPKHAB; ISSN: 0044-4618

DOCUMENT TYPE: Journal

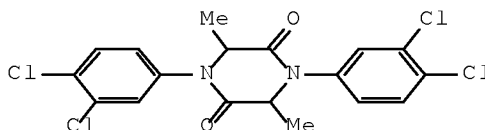
LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 105:97894

GI



I



II

AB Thermal stabilities of N-aryl-substituted amino acids I (R = H, Cl, MeO; R1 = H, Cl, Me; R2 = H, Cl, Me, MeO, EtO; R3 = H, Cl; R4 = H, Me, EtO) were studied by DTA at 120-40°. I having halo substituents on the benzene ring are most stable. I having alkyl or alkoxy groups on the benzene ring generally melt

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with decomposition dimeric compound II was formed in the thermolysis of the Na salt of I (R = R3 = H, R1 = R2 = Cl, R4 = Me).

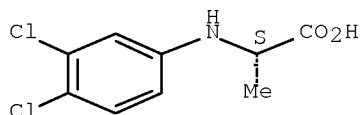
IT 103678-29-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal stability of)

RN 103678-29-1 ZCAPLUS

CN L-Alanine, N-(3,4-dichlorophenyl)-, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Na

L58 ANSWER 63 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:615799 ZCAPLUS Full-text

DOCUMENT NUMBER: 103:215799

ORIGINAL REFERENCE NO.: 103:34803a,34806a

TITLE: Practical stereospecific production of optically active α -aminocarboxylic acid esters
INVENTOR(S): Drauz, Karlheinz; Burkard, Ulrike; Effenberger, Franz
PATENT ASSIGNEE(S): Degussa A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 50 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3328986	A1	19850221	DE 1983-3328986	19830811
EP 134392	A1	19850320	EP 1984-103638	19840403
R: BE, CH, DE, FR, GB, LI				
JP 60058950	A	19850405	JP 1984-166658	19840810
PRIORITY APPLN. INFO.:			DE 1983-3328986	A 19830811

OTHER SOURCE(S): CASREACT 103:215799; MARPAT 103:215799

AB Optically active α -amino acid esters were prepared by condensation of optically active O-(trifluoromesyl)lactic acid esters with the appropriate amines. Thus, reaction of 24.24 g 2,6-Me2C6H3NH2 with (S)-F3CS(O)2OCHMeCO2Me in CH2Cl at 25° for 17 h gave (R)-2,6-Me2C6H3NHCHMeCO2Me.

IT 62840-19-1P

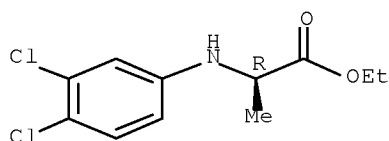
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 62840-19-1 ZCAPLUS

CN D-Alanine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

10/598508



L58 ANSWER 64 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:591466 ZCAPLUS Full-text

DOCUMENT NUMBER: 103:191466

ORIGINAL REFERENCE NO.: 103:30732h,30733a

TITLE: Alanine derivatives as plant growth regulators

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60109504	A	19850615	JP 1983-217166	19831118
US 4619685	A	19861028	US 1984-671689	19841115
CA 1287231	C	19910806	CA 1984-468098	19841116
PRIORITY APPLN. INFO.:			JP 1983-217166	A 19831118

OTHER SOURCE(S): CASREACT 103:191466; MARPAT 103:191466

AB N-Substituted alanine derivs. are plant growth regulators especially effective in controlling axillary bud growth in tobacco and lodging in cereals. Syntheses are described. Thus, 2000 ppm N-(3-chloro-4-fluorophenyl)alanine Et ester [83442-76-6] controlled axillary bud growth in tobacco and lodging in rice.

IT 52756-24-8P 83442-76-6P 98926-57-9P

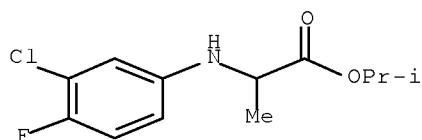
98926-58-0P 98926-64-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and phytohormone activity of)

RN 52756-24-8 ZCAPLUS

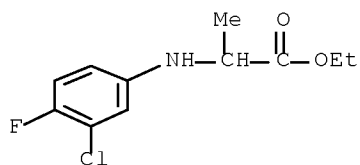
CN Alanine, N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester (CA INDEX NAME)



RN 83442-76-6 ZCAPLUS

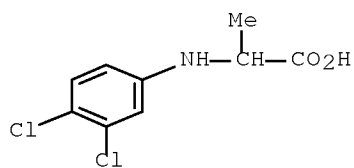
CN Alanine, N-(3-chloro-4-fluorophenyl)-, ethyl ester (CA INDEX NAME)

10/598508



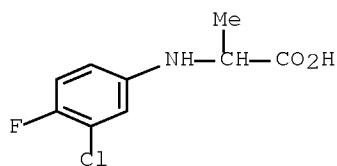
RN 98926-57-9 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, monosodium salt (9CI) (CA INDEX NAME)



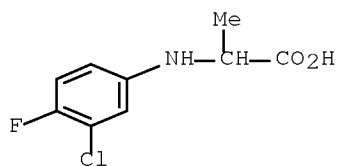
RN 98926-58-0 ZCAPLUS

CN Alanine, N-(3-chloro-4-fluorophenyl)-, monosodium salt (9CI) (CA INDEX NAME)



RN 98926-64-8 ZCAPLUS

CN Alanine, N-(3-chloro-4-fluorophenyl)-, monopotassium salt (9CI) (CA INDEX NAME)



L58 ANSWER 65 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:483545 ZCAPLUS Full-text
 DOCUMENT NUMBER: 103:83545
 ORIGINAL REFERENCE NO.: 103:13377a,13380a
 TITLE: Pest control
 INVENTOR(S): Lyr, Horst; Otto, Dieter; Strumpf, Thomas; Weber, Bernd
 PATENT ASSIGNEE(S): Akademie der Landwirtschaftswissenschaften der DDR, Institut fuer Pflanzenschutzforschung, Ger. Dem. Rep.
 SOURCE: Ger. (East), 19 pp.
 CODEN: GEXXA8
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DD 219374	A1	19850306	DD 1983-255883	19831024
PRIORITY APPLN. INFO.:			DD 1983-255883	19831024

AB Compns. containing knowns carboxylic acid insecticides, es. pyrethroids, such as fenvalerate [51630-58-1], permethrin [52645-53-1] or decamethrin [52918-63-5], and known acylaniline fungicides, such as CGA 29212 [52888-51-4], are synergistic. Thus, fenvalerate plus N-(2,6-dimethylphenyl)-N-(2-furoyl)alanine Me ester [79048-45-6] showed synergistic toxicity to *Musca domestica*, in the laboratory

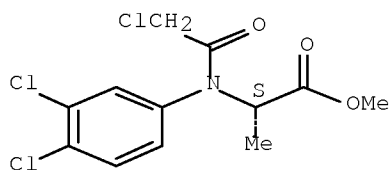
IT 97716-91-1

RL: BIOL (Biological study)
 (insecticidal composition containing, synergistic)

RN 97716-91-1 ZCAPLUS

CN L-Alanine, N-(chloroacetyl)-N-(3,4-dichlorophenyl)-, methyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 66 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:156983 ZCAPLUS Full-text
 DOCUMENT NUMBER: 100:156983
 ORIGINAL REFERENCE NO.: 100:23931a,23934a
 TITLE: Substituted anilino acids
 INVENTOR(S): Simon-Bierenbaum, R.; Ertley, Ernest W.; Goetz, Frederick J.; Tang, David Y.
 PATENT ASSIGNEE(S): Occidental Chemical Corp., USA
 SOURCE: U.S., 8 pp.
 CODEN: USXXAM

10/598508

DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4424396	A	19840103	US 1982-400219	19820721
PRIORITY APPLN. INFO.:			US 1982-400219	19820721
OTHER SOURCE(S):	CASREACT 100:156983; MARPAT 100:156983			
GI				



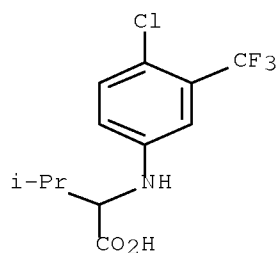
AB Anilino acids (I; R = H, metal cation; R1 = H, C1-5 alkyl, C2-5 alkenyl, C1-4 haloalkyl, C2-4 haloalkenyl, C3-4 cycloalkyl; Y = H, Cl, Me, CF3; X = H, Cl, F) were prepared by reacting a corresponding aryl halide with an α -amino acid, R1CH(NH2)CO2R. Thus, a mixture of 3,4-dichlorobenzotrifluoride, potassium valinate, and sulfolane was heated and maintained at about 160° for .apprx.48 h, with mixing to give I (R = H, R1 = Me2CH, X = 2-Cl, Y = 4-CF3) in 65% yield.

IT 69411-31-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 69411-31-0 ZCAPLUS

CN Valine, N-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L58 ANSWER 67 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:85354 ZCAPLUS Full-text

DOCUMENT NUMBER: 100:85354

ORIGINAL REFERENCE NO.: 100:12933a,12936a

TITLE: Synthesis of derivatives of N,N-substituted thiolcarbamates

AUTHOR(S): Kamynina, V. F.; Savin, V. P.

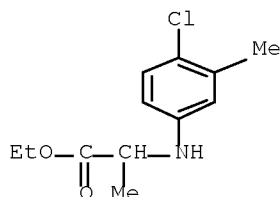
CORPORATE SOURCE: USSR

SOURCE: Pestitsidy i ikh Primenenie, M. (1983) 15-17
 From: Ref. Zh., Khim. 1983, Abstr. No. 210298

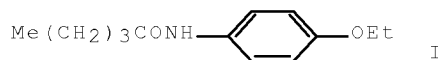
DOCUMENT TYPE: Journal

10/598508

LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 100:85354
AB Title only translated.
IT 88912-00-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et chlorothiocarbonate)
RN 88912-00-9 ZCAPLUS
CN Alanine, N-(4-chloro-3-methylphenyl)-, ethyl ester (CA INDEX NAME)



L58 ANSWER 68 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:63391 ZCAPLUS Full-text
DOCUMENT NUMBER: 100:63391
ORIGINAL REFERENCE NO.: 100:9597a,9600a
TITLE: Search for synergists to herbicide preparations. 1.
Potential synergists for karakhol and 2,4-D
AUTHOR(S): Lyapkova, N. V.; Semenov, V. A.; Bazunova, G. G.;
Mikhailova, G. V.; Davydov, A. M.; Antipanova, V. E.;
Novak, N. V.; Kamynina, V. F.
CORPORATE SOURCE: VNII Gerbitsidov Regulyatorov Rosta Rasten., USSR
SOURCE: Agrokhimiya (1983), (11), 101-5
CODEN: AGKYAU; ISSN: 0002-1881
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

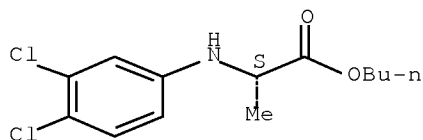


AB Of 8 potential synergists of 0.5 kg Karakhol [33878-50-1]/ha, 0.5 kg N-4-ethoxyphenylvaleramide (I) [88552-40-3] and N-4-ethoxy-2-methylphenylvaleramide [88552-41-4]/ha were the most effective, synergizing the inhibition of Avena fatua growth by 18 and 12%, resp. The synergists alone did not affect the A. fatua growth. Of 7 potential synergists of 0.1 kg 2,4-D amine [2008-39-1]/ha, 0.1 kg Me 3-(methoxycarbonylmethylthio)propionate [7400-45-5] and Bu 3-(butoxycarbonylmethylthio)propionate [88552-43-6]/ha were the most effective, synergizing the inhibition of sunflower growth by 37 and 30%, resp. The synergists alone inhibited the sunflower growth by $\leq 10\%$. Syntheses were given.
IT 71267-80-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et thiochlorocarbonate)

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RN 71267-80-6 ZCAPLUS
CN L-Alanine, N-(3,4-dichlorophenyl)-, butyl ester (CA INDEX NAME)

Absolute stereochemistry.

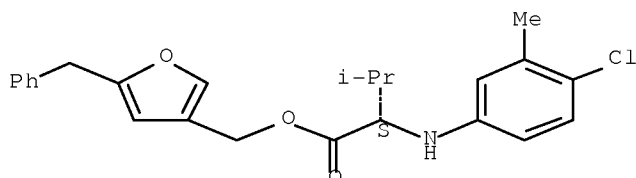


L58 ANSWER 69 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:558033 ZCAPLUS Full-text
DOCUMENT NUMBER: 99:158033
ORIGINAL REFERENCE NO.: 99:24217a,24220a
TITLE: Anilinoacetates
PATENT ASSIGNEE(S): Dainippon Jochugiku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58116442	A	19830711	JP 1982-130067	19820726
JP 61023179	B	19860604		

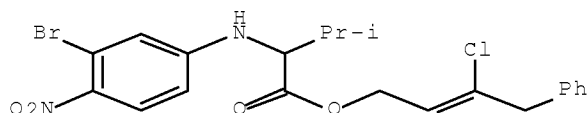
PRIORITY APPLN. INFO.: JP 1982-130067 19820726
AB RNHCHR1CO2R2 [I: R = (substituted) phenyl; R1 = (substituted) alkyl, alkenyl, alkynyl, etc.; R2 = substituted cycloalkenylmethyl, substituted heterocyclylmethyl] were prepared Thus, heating 4.9 g the acid chloride of I (R = 3,4-Me2C6H3, R1 = Me2CH, R2 = H) in benzene containing pyridine with 4.2 g 5-phenoxy-2-thenyl alc. at 50° gave 7.1 g I (R = 3,4-Me2C6H3, R1 = Me2CH, R2 = 5-phenoxy-2-thenyl). The insecticidal activities of I were comparable to that of allethrin.
IT 64823-65-0P 84600-06-6P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and insecticidal activity of)
RN 64823-65-0 ZCAPLUS
CN L-Valine, N-(4-chloro-3-methylphenyl)-, [5-(phenylmethyl)-3-furanyl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.



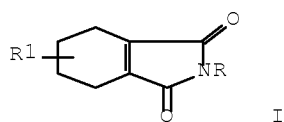
10/598508

RN 84600-06-6 ZCAPLUS
 CN Valine, N-(3-bromo-4-nitrophenyl)-, 3-chloro-4-phenyl-2-butenyl ester
 (9CI) (CA INDEX NAME)



L58 ANSWER 70 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1983:522298 ZCAPLUS Full-text
 DOCUMENT NUMBER: 99:122298
 ORIGINAL REFERENCE NO.: 99:18833a,18836a
 TITLE: N-(3-Substituted aminophenyl)tetrahydrophthalimides
 and herbicidal composition
 INVENTOR(S): Jukihara, Tetsuo; Ushinohama, Kazuyuki; Natsume,
 Bunzi; Watanabe, Hisao; Suzuki, Seiichi
 PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd. , Japan
 SOURCE: Eur. Pat. Appl., 130 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 77938	A2	19830504	EP 1982-109201	19821005
EP 77938	A3	19830824		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 58072562	A	19830430	JP 1981-169846	19811023
JP 58103363	A	19830620	JP 1981-199847	19811211
JP 02057543	B	19901205		
ZA 8207487	A	19830831	ZA 1982-7487	19821013
AU 8289463	A	19830428	AU 1982-89463	19821018
HU 30857	A2	19840428	HU 1982-3362	19821021
DK 8204700	A	19830424	DK 1982-4700	19821022
BR 8206186	A	19830920	BR 1982-6186	19821022
ES 516765	A1	19831201	ES 1982-516765	19821022
PRIORITY APPLN. INFO.:			JP 1981-169846	A 19811023
			JP 1981-199847	A 19811211
OTHER SOURCE(S):			CASREACT 99:122298; MARPAT 99:122298	
GI				

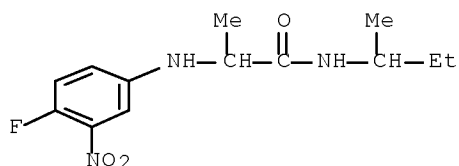


AB Phthalimides I (R = substituted 3-aminophenyl; R1 = H, Me) (366 compds.) were prepared Thus, 1,2-cyclohexenedicarboxylic anhydride was treated with 4-chloro-2-fluoro-5-nitroaniline and then hydrogenated in the presence of Pd-C to give I (R = 5-amino-4-chloro-2-fluorophenyl, R1 = H) which at 6.25 g/a preemergence gave >90% control of, e.g., *Chenopodium album*.

IT 86988-04-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of)

RN 86988-04-7 ZCAPLUS

CN Propanamide, 2-[(4-fluoro-3-nitrophenyl)amino]-N-(1-methylpropyl)- (CA INDEX NAME)



L58 ANSWER 71 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1983:102714 ZCAPLUS Full-text

DOCUMENT NUMBER: 98:102714

ORIGINAL REFERENCE NO.: 98:15597a,15600a

TITLE: Insecticide composition

PATENT ASSIGNEE(S): Dainippon Jochugiku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKXXAF

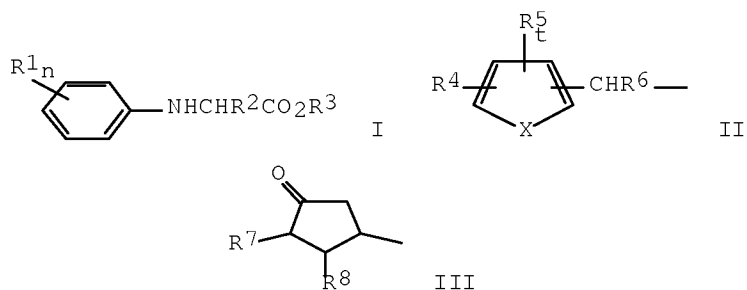
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57171903	A	19821022	JP 1982-50402	19820329
JP 59043924	B	19841025		
PRIORITY APPLN. INFO.: GI			JP 1982-50402	19820329

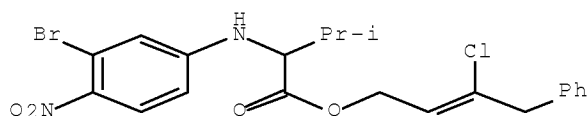


AB The compds. I (R' = H, halo, alkyl, alkenyl, etc.; R2 = alkyl, alkenyl, etc.; n = 1-3; R3 = II, III, where R4 = H, allyl, propargyl, benzyl, etc., R5 = H, Me, halo, etc., t = 1-2, R6 = H, ethynyl, or cyano, X = O, S, etc., R7 = allyl, propargyl, benzyl, or pentadiene, R8 = H or Me, etc.) are insecticides. Syntheses of I are described. Thus, 0.2% 5'-propargyl-2'-methyl-3'-flurylmethyl- α -isopropyl-(m- acetylanilino)acetate [84600-02-2] controlled houseflies.

IT 84600-06-6P 84600-12-4P
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and insecticidal activity of)

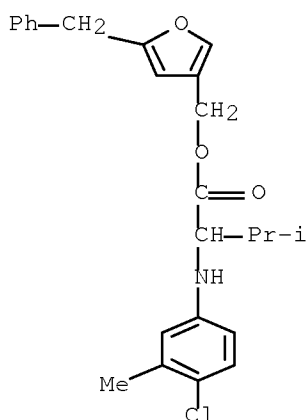
RN 84600-06-6 ZCAPLUS

CN Valine, N-(3-bromo-4-nitrophenyl)-, 3-chloro-4-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)



RN 84600-12-4 ZCAPLUS

CN Valine, N-(4-chloro-3-methylphenyl)-, [5-(phenylmethyl)-3-furanyl]methyl ester (CA INDEX NAME)



L58 ANSWER 72 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1983:102691 ZCAPLUS Full-text

DOCUMENT NUMBER: 98:102691

ORIGINAL REFERENCE NO.: 98:15593a,15596a

TITLE: Phenylamino acid derivatives as herbicides

PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan

10/598508

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57116003	A	19820719	JP 1981-2738	19810113
PRIORITY APPLN. INFO.:			JP 1981-2738	19810113

OTHER SOURCE(S): CASREACT 98:102691

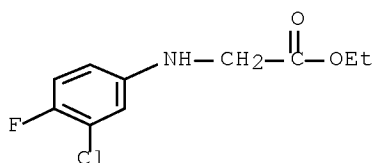
AB N-Substituted phenylamino acids are herbicides. Synthesis of the compds. is described. Thus, N-(3,4-dichlorophenyl)glycine [5465-90-7] (20 g/are) controlled Echinochloa crus-galli, Scirpus hotarui, Sagittaria pygmaea, and other broadleaf weeds in rice.

IT 2344-98-1F 31399-32-3P 83442-58-4F
 83442-68-6P 83442-76-6P 83442-80-2P
 83442-84-6P 83442-86-8P 83442-92-6P
 83448-40-2P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and herbicidal activity of)

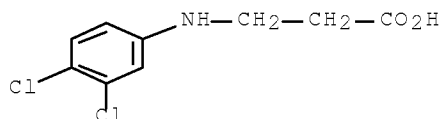
RN 2344-98-1 ZCAPLUS

CN Glycine, N-(3-chloro-4-fluorophenyl)-, ethyl ester (CA INDEX NAME)



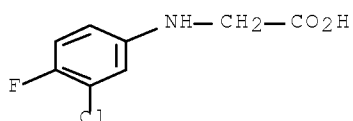
RN 31399-32-3 ZCAPLUS

CN β-Alanine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)



RN 83442-58-4 ZCAPLUS

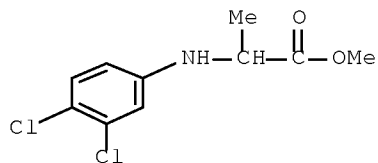
CN Glycine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)



10/598508

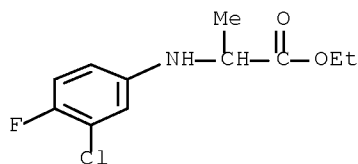
RN 83442-68-6 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)



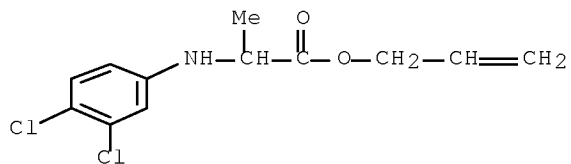
RN 83442-76-6 ZCAPLUS

CN Alanine, N-(3-chloro-4-fluorophenyl)-, ethyl ester (CA INDEX NAME)



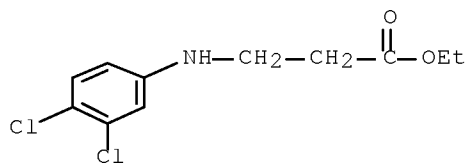
RN 83442-80-2 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, 2-propenyl ester (9CI) (CA INDEX NAME)



RN 83442-84-6 ZCAPLUS

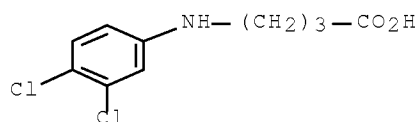
CN β-Alanine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)



10/598508

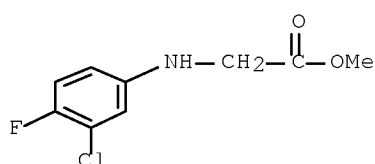
RN 83442-86-8 ZCAPLUS

CN Butanoic acid, 4-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



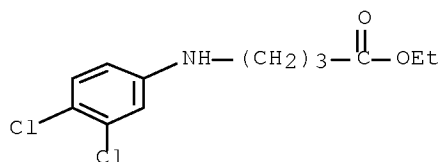
RN 83442-92-6 ZCAPLUS

CN Glycine, N-(3-chloro-4-fluorophenyl)-, methyl ester (CA INDEX NAME)



RN 83448-40-2 ZCAPLUS

CN Butanoic acid, 4-[(3,4-dichlorophenyl)amino]-, ethyl ester (CA INDEX NAME)



L58 ANSWER 73 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:123297 ZCAPLUS Full-text

DOCUMENT NUMBER: 96:123297

ORIGINAL REFERENCE NO.: 96:20265a,20268a

TITLE: Substituted amino acids

INVENTOR(S): Henrick, Clive A.; Garcia, Barbara A.

PATENT ASSIGNEE(S): Zoecon Corp., USA

SOURCE: U.S., 23 pp. Cont.-in-part of U.S. Ser. No. 824,947, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.

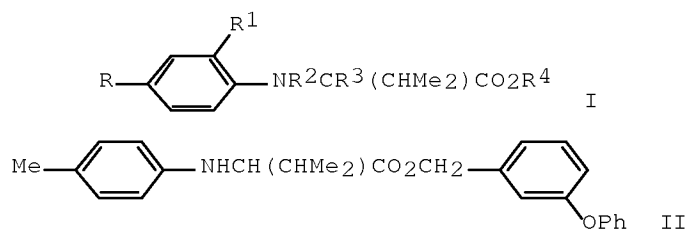
KIND

DATE

APPLICATION NO.

DATE

US 4243819	A	19810106	US 1978-878091	19780216
ZA 7801173	A	19790228	ZA 1978-1173	19780228
GB 1588111	A	19810415	GB 1978-9026	19780307
CA 1147745	A1	19830607	CA 1978-298515	19780308
IN 148104	A1	19801018	IN 1978-CA264	19780313
IL 54293	A	19820831	IL 1978-54293	19780315
AU 7834253	A	19790920	AU 1978-34253	19780317
AU 519047	B2	19811105		
ES 468013	A1	19781201	ES 1978-468013	19780318
DE 2812169	A1	19781005	DE 1978-2812169	19780320
DE 2812169	C2	19911017		
JP 53121731	A	19781024	JP 1978-32263	19780320
JP 62003146	B	19870123		
BR 7801712	A	19781219	BR 1978-1712	19780320
FR 2405922	A1	19790511	FR 1978-8047	19780320
FR 2405922	B1	19840330		
CH 632232	A5	19820930	CH 1978-3021	19780320
BE 865114	A1	19780921	BE 1978-186111	19780321
DK 7801272	A	19780922	DK 1978-1272	19780321
DK 154642	B	19881205		
DK 154642	C	19890619		
NL 7803030	A	19780925	NL 1978-3030	19780321
NL 193021	B	19980401		
NL 193021	C	19980804		
FR 2392959	A1	19781229	FR 1978-24616	19780824
US 4231953	A	19801104	US 1979-45565	19790604
US 4252724	A	19810224	US 1979-66264	19790813
US 4411912	A	19831025	US 1979-93553	19791113
PRIORITY APPLN. INFO.:			US 1977-779886	A2 19770321
			US 1977-824947	A2 19770815
			US 1978-878091	A 19780216
OTHER SOURCE(S):	CASREACT 96:123297; MARPAT 96:123297			
GI				



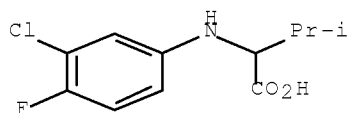
- AB N-Ph amino acids I (R = C1-4 alkyl, Cl, F, Br, CF₃, C1-4 alkylcarbonyl, cyclopropyl, C1-4 alkylthio optionally substituted with halo; R₁ = H, CF₃, F, Cl, Br, C1-4 alkoxy, C1-3 alkylthio, C1-4 alkyl; R₂ = H, Me, Et; R₃ = H, F; R₄ = H, metal cation) were prepared as pesticides. Thus, Me₂CHCHBrCO₂H was treated with SOCl₂ to give the acid chloride, which was esterified with m-(PhO)C₆H₄CH₂OH to give the ester, which was treated with p-toluidine to give valine II. II gave a LC₅₀ <0.01% when tested as an insecticide against *Musca domestica* L.
- IT 69410-21-5 69410-70-4 69411-31-0
69411-58-1

10/598508

RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with phenoxybenzyl bromide)

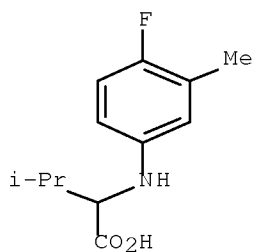
RN 69410-21-5 ZCAPLUS

CN Valine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)



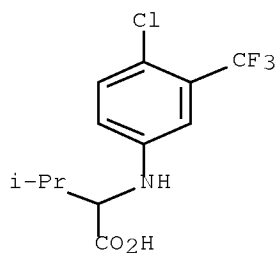
RN 69410-70-4 ZCAPLUS

CN Valine, N-(4-fluoro-3-methylphenyl)- (CA INDEX NAME)



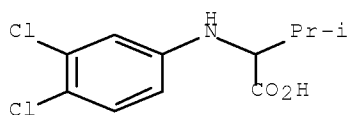
RN 69411-31-0 ZCAPLUS

CN Valine, N-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



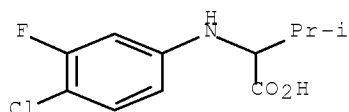
RN 69411-58-1 ZCAPLUS

CN Valine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)

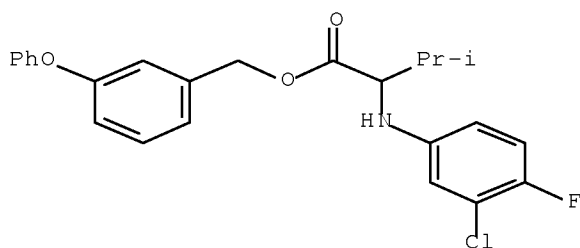


10/598508

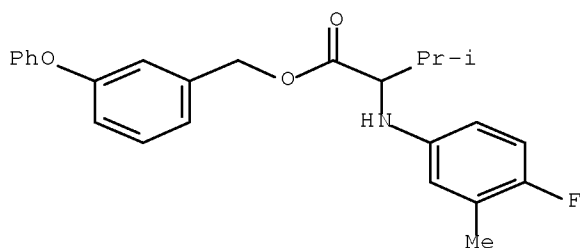
IT 69411-82-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and esterification of, with phenoxybenzyl bromide)
RN 69411-82-1 ZCAPLUS
CN Valine, N-(4-chloro-3-fluorophenyl)- (CA INDEX NAME)



IT 69410-22-6P 69410-71-5P 69411-34-3P
69411-59-2P 69411-87-6P 69411-91-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 69410-22-6 ZCAPLUS
CN Valine, N-(3-chloro-4-fluorophenyl)-, (3-phenoxyphenyl)methyl ester (CA
INDEX NAME)

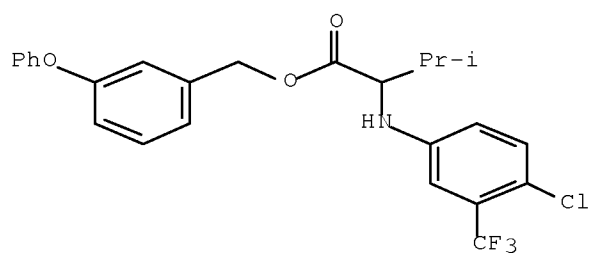


RN 69410-71-5 ZCAPLUS
CN Valine, N-(4-fluoro-3-methylphenyl)-, (3-phenoxyphenyl)methyl ester (CA
INDEX NAME)

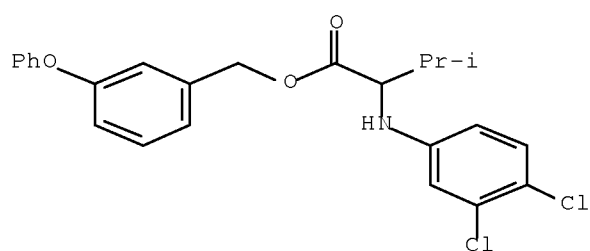


RN 69411-34-3 ZCAPLUS
CN Valine, N-[4-chloro-3-(trifluoromethyl)phenyl]-, (3-phenoxyphenyl)methyl
ester (CA INDEX NAME)

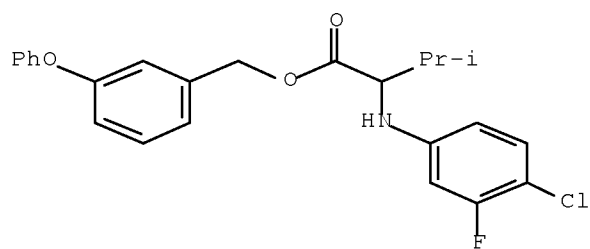
10/598508



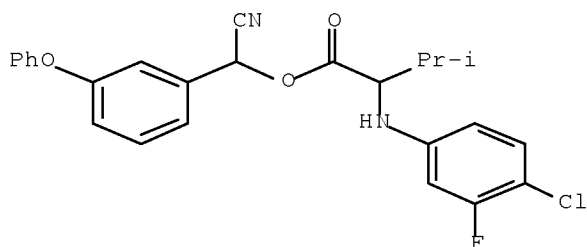
RN 69411-59-2 ZCAPLUS
CN Valine, N-(3,4-dichlorophenyl)-, (3-phenoxyphenyl)methyl ester (CA INDEX NAME)



RN 69411-87-6 ZCAPLUS
CN Valine, N-(4-chloro-3-fluorophenyl)-, (3-phenoxyphenyl)methyl ester (CA INDEX NAME)



RN 69411-91-2 ZCAPLUS
CN Valine, N-(4-chloro-3-fluorophenyl)-, cyano(3-phenoxyphenyl)methyl ester (CA INDEX NAME)



L58 ANSWER 74 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:169431 ZCAPLUS Full-text

DOCUMENT NUMBER: 94:169431

ORIGINAL REFERENCE NO.: 94:27643a,27646a

TITLE: Synergetic herbicide composition containing an aromatic amine compound

INVENTOR(S): Clayton, Anthony Broxholme; Lehman, Stanley Keith

PATENT ASSIGNEE(S): Hercules Inc., USA

SOURCE: Rom., 19 pp.
CODEN: RUXXA3

DOCUMENT TYPE: Patent

LANGUAGE: Romanian

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RO 69046	A1	19801030	RO 1973-86865	19730310
CA 1013960	A1	19770719	CA 1973-160333	19730102
CA 1257608	A1	19890718	CA 1973-160332	19730102
ZA 7300316	A	19731031	ZA 1973-316	19730116
AU 7351831	A	19740808	AU 1973-51831	19730205
DK 140082	C	19791119	DK 1973-725	19730209
DK 140082	B	19791119		
ES 411527	A3	19760101	ES 1973-411527	19730212
JP 49000232	A	19740105	JP 1973-20314	19730221
BE 796263	A1	19730702	BE 1973-128358	19730305
GB 1417273	A	19751210	GB 1973-10971	19730307
FR 2176075	A1	19731026	FR 1973-9209	19730308
FR 2176075	B1	19790511		
NL 7303363	A	19730912	NL 1973-3363	19730309
NL 178248	B	19850916		
NL 178248	C	19860217		
IT 981287	B	19741010	IT 1973-21429	19730309
IT 981288	B	19741010	IT 1973-21430	19730309
CH 578830	A5	19760831	CH 1973-3525	19730309
AT 7302088	A	19770215	AT 1973-2088	19730309
AT 339284	B	19771010		
HU 170006	B	19770328	HU 1973-HE628	19730309
CH 602594	A5	19780731	CH 1975-7022	19730309
SU 1001847	A3	19830228	SU 1973-1894761	19730309
JP 48099341	A	19731215	JP 1973-28471	19730310
PL 94343	B1	19770730	PL 1973-161187	19730310
PL 100047	B1	19780831	PL 1973-191942	19730310
PL 101581	B1	19790131	PL 1973-201129	19730310
PL 101587	B1	19790131	PL 1973-201130	19730310

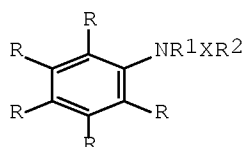
10/598508

RO 68549	A1	19810924	RO 1973-74131	19730310
RO 69047	A1	19820510	RO 1973-86866	19730310
SE 411206	B	19750212	SE 1975-1572	19750212
SE 411206	C	19800327		
SE 7510667	A	19750923	SE 1975-10667	19750923
AT 349827	B	19790212	AT 1975-8102	19751023
AT 7803708	A	19800115	AT 1978-3708	19780522
AT 358322	B	19800910		
AT 7803707	A	19800915	AT 1978-3707	19780522
AT 362185	B	19810427		
AT 8003146	A	19801115	AT 1980-3146	19800613
AT 362958	B	19810625		
AT 8003147	A	19801115	AT 1980-3147	19800613
AT 362959	B	19810625		

PRIORITY APPLN. INFO.:

US 1972-233817	A	19720310
US 1972-233818	A	19720310
AT 1973-2088	A	19730309
CH 1973-3525	A	19730309

GI



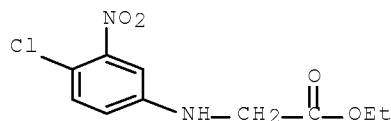
AB Synergistic herbicidal compns are given, containing the anilines I (R = H, halo, NO₂, trihalomethyl, Cl-7 alkyl or alkoxy; R₁ = H or haloacetyl; X = alkylene or alkylidene; R₂ = CO₂H, CONH₂, substituted amide, alkoxy carbonyl, etc.) and pyrazon [1698-60-8]. Thus, a composition containing N-chloroacetyl-N-(2,6-diethylphenyl)glycine Et ester [38727-55-8] (2.2 kg/ha) and 4.4 kg pyrazon/ha, applied postemergence, totally controlled Chenopodium and other weeds, with no phytotoxicity to sugar beet, whereas the components by themselves were less active.

IT 51114-23-9P 51114-28-4P 51114-31-9P
 51114-36-4P 51114-38-6P 51114-41-1P
 51114-44-4P 77325-93-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and synergistic herbicidal activity of)

RN 51114-23-9 ZCAPLUS

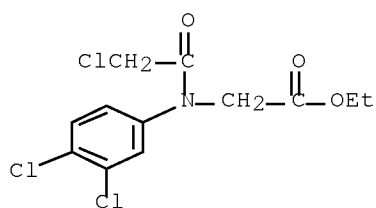
CN Glycine, N-(4-chloro-3-nitrophenyl)-, ethyl ester (CA INDEX NAME)



RN 51114-28-4 ZCAPLUS

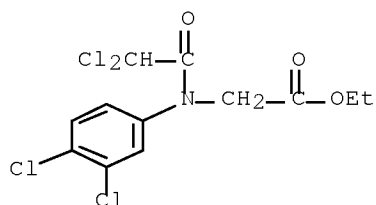
CN Glycine, N-(chloroacetyl)-N-(3,4-dichlorophenyl)-, ethyl ester (9CI) (CA INDEX NAME)

10/598508



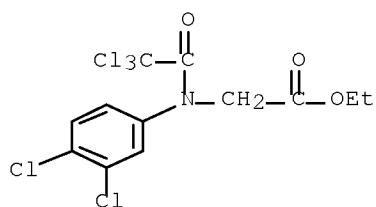
RN 51114-31-9 ZCAPLUS

CN Glycine, N-(dichloroacetyl)-N-(3,4-dichlorophenyl)-, ethyl ester (9CI)
(CA INDEX NAME)



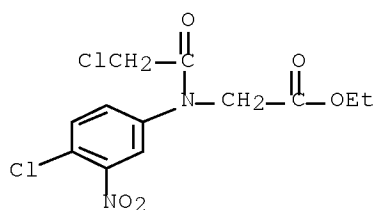
RN 51114-36-4 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)-N-(trichloroacetyl)-, ethyl ester (9CI)
(CA INDEX NAME)



RN 51114-38-6 ZCAPLUS

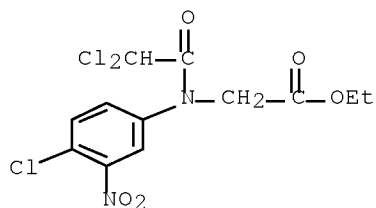
CN Glycine, N-(chloroacetyl)-N-(4-chloro-3-nitrophenyl)-, ethyl ester (9CI)
(CA INDEX NAME)



10/598508

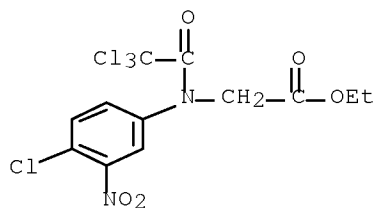
RN 51114-41-1 ZCAPLUS

CN Glycine, N-(4-chloro-3-nitrophenyl)-N-(dichloroacetyl)-, ethyl ester (9CI)
(CA INDEX NAME)



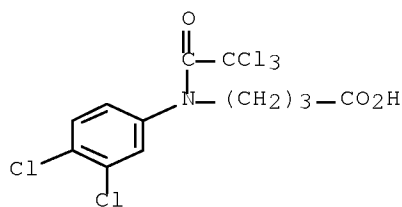
RN 51114-44-4 ZCAPLUS

CN Glycine, N-(4-chloro-3-nitrophenyl)-N-(trichloroacetyl)-, ethyl ester
(9CI) (CA INDEX NAME)



RN 77325-93-0 ZCAPLUS

CN Butanoic acid, 4-[(3,4-dichlorophenyl)(trichloroacetyl)amino]- (9CI) (CA
INDEX NAME)



L58 ANSWER 75 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:169427 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 94:169427

ORIGINAL REFERENCE NO.: 94:27643a,27646a

TITLE: Plant growth regulating composition containing

10/598508

substituted anilinoalkanoic acid esters
 INVENTOR(S): Creuzburg, Doerthe; Kleiner, Ralf; Kochmann, Werner;
 Lang, Sieghard; Naumann, Kurt; Toepfer, Roswitha
 PATENT ASSIGNEE(S): VEB Chemiekombinat Bitterfeld, Ger. Dem. Rep.
 SOURCE: Ger. (East), 15 pp.
 CODEN: GEXXA8
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 142276	A1	19800618	DD 1979-211638	19790319

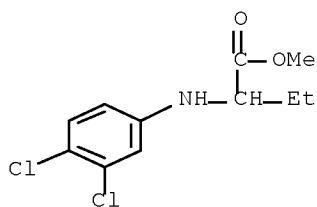
PRIORITY APPLN. INFO.: DD 1979-211638 A1 19790319

AB The anilinoalkanoic acid esters RNR1CH₂CO₂R₂ (R = Ph, substituted Ph, PhNH, cyclohexyl, etc.; R₁ = H, cycloalkyl, etc.; R₂ = H alkyl, or alkali metal) are plant growth regulators. Thus, 0.05-0.4% PhC₂H₄CO₂Me [77165-36-7] increased the fresh weight of wheat shoots.

IT 77165-31-2
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study);
 USES (Uses)
 (plant growth regulator)

RN 77165-31-2 ZCAPLUS

CN Butanoic acid, 2-[(3,4-dichlorophenyl)amino]-, methyl ester (CA INDEX NAME)



L58 ANSWER 76 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1981:121712 ZCAPLUS Full-text
 DOCUMENT NUMBER: 94:121712
 ORIGINAL REFERENCE NO.: 94:19915a,19918a
 TITLE: Herbicidal N-arylcarbamoylmethyl
 (di)thiophosphoric(phosphonic) acid esters(amides)
 INVENTOR(S): Salbeck, Gerhard; Koch, Manfred; Mildenerberger, Hilmar;
 Bieringer, Hermann; Koecher, Helmut
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 26 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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10/598508

DE 2908739	A1	19800918	DE 1979-2908739	19790306
EP 16363	A1	19801001	EP 1980-101035	19800303

R: AT, BE, CH, DE, FR, GB, IT, NL

DK 8000945	A	19800907	DK 1980-945	19800305
AU 8056152	A	19800911	AU 1980-56152	19800305
JP 55118493	A	19800911	JP 1980-26810	19800305
BR 8001304	A	19801104	BR 1980-1304	19800305

PRIORITY APPLN. INFO.: DE 1979-2908739 A 19790306

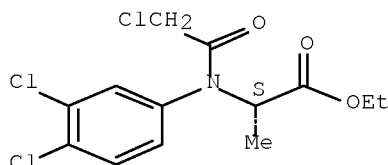
AB Thirty title compds., $R_nC_6H_5-nN(CHR_3CO_2R_4)COCH_2SP(X)(OR_2)R_1$ [I, R = halo, alkyl, alkoxy, haloalkyl, alkylthio, NO₂, aryloxy; R₁ = alkyl, CH₂Cl, alkoxy, alkylamino, alkyleneamino, heterocyclyl, alkylthio; R₂ = alkyl; R₃ = H, alkyl; R₄ = H, alkyl, alkoxycarbonyl, alkoxy, alkylthio, alkylamino, oxiranyl, phenoxy, alkenyl, alkynyl, furyl; X = O, S; n = 1-3] were prepared by esterification of $R_nC_6H_5-nN(CHR_3CO_2R_4)COCH_2Cl$ with $R_1(R_2O)P(X)OM$ (M = SNH₄, SNa). Herbicidal data were given for I. E.g., I (R_n = 2,6-Et₂, R₁ = OEt, R₂ = R₄ = Et, R₃ = H, X = S) at 2.4 kg AS/ha gave 100% kill of Echinochloa, Setaria and Amaranthus.

IT 76814-65-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (esterification of, with phosphorus acid derivs.)

RN 76814-65-8 ZCAPLUS

CN L-Alanine, N-(chloroacetyl)-N-(3,4-dichlorophenyl)-, ethyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 77 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:616683 ZCAPLUS Full-text

DOCUMENT NUMBER: 93:216683

ORIGINAL REFERENCE NO.: 93:34523a,34526a

TITLE: Algicidal product containing diamines

INVENTOR(S): Van Gilse, Jaap; Paerels, Gerard Bernard

PATENT ASSIGNEE(S): Duphar International Research B. V., Neth.

SOURCE: Fr. Demande, 43 pp.
 CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

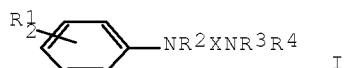
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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FR 2437785	A1	19800430	FR 1979-19298	19790726
FR 2437785	B1	19840629		
NL 7905235	A	19800129	NL 1979-5235	19790705
ZA 7903568	A	19810225	ZA 1979-3568	19790716
DE 2929181	A1	19800214	DE 1979-2929181	19790719
DK 7903091	A	19800127	DK 1979-3091	19790723

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SE 7906293	A	19800128	SE 1979-6293	19790723
IL 57868	A	19820831	IL 1979-57868	19790723
BE 877867	A1	19800124	BE 1979-196436	19790724
ES 482799	A1	19800901	ES 1979-482799	19790724
DD 145049	A5	19801119	DD 1979-214604	19790725
HU 24063	A2	19821228	HU 1979-DU311	19790725
JP 55019300	A	19800209	JP 1979-95565	19790726
JP 63020801	B	19880430		
AU 7949687	A	19800501	AU 1979-49687	19790808
AU 526440	B2	19830113		
ES 490775	A1	19801201	ES 1980-490775	19800422
PRIORITY APPLN. INFO.:			NL 1978-7908	A 19780726
GI				

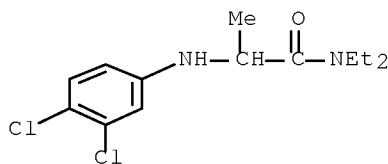


AB The diamines I (R1 = halo, alkyl, alkoxy, etc; R2 = H, alkyl, etc.; X = alkylene; R3 = H or C1-4 alkyl; R4 = C1-6 alkyl; R3R4 = polymethylene) and related compds. are algicides. Thus, N-(3,4-dichlorophenyl)-N,N'-diethylethylenediamine [74473-98-6] (2 mg/L) totally controlled Vaucheria, Claudospora, Mougeotia, and Eudogonium. The synthesis of the compds. is given.

IT 74474-39-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of)

RN 74474-39-8 ZCAPLUS

CN Propanamide, 2-[(3,4-dichlorophenyl)amino]-N,N-diethyl- (CA INDEX NAME)



L58 ANSWER 78 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:463603 ZCAPLUS Full-text

DOCUMENT NUMBER: 93:63603

ORIGINAL REFERENCE NO.: 93:10299a,10302a

TITLE: Algicidal compositions

INVENTOR(S): Van Gilse, Jaap; Paerels, Gerard Bernard

PATENT ASSIGNEE(S): Duphar International Research B. V., Neth.

SOURCE: Brit. UK Pat. Appl., 26 pp.
 CODEN: BAXXDU

DOCUMENT TYPE: Patent

LANGUAGE: English

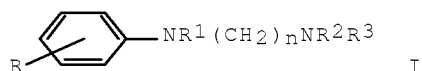
FAMILY ACC. NUM. COUNT: 3

10/598508

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2026867	A	19800213	GB 1979-25573	19790723
GB 2026867	B	19820908		
NL 7905235	A	19800129	NL 1979-5235	19790705
ZA 7903568	A	19810225	ZA 1979-3568	19790716
DE 2929181	A1	19800214	DE 1979-2929181	19790719
DK 7903091	A	19800127	DK 1979-3091	19790723
SE 7906293	A	19800128	SE 1979-6293	19790723
GB 2072188	A	19810930	GB 1981-9842	19790723
GB 2072188	B	19830316		
IL 57868	A	19820831	IL 1979-57868	19790723
BE 877867	A1	19800124	BE 1979-196436	19790724
ES 482799	A1	19800901	ES 1979-482799	19790724
DD 145049	A5	19801119	DD 1979-214604	19790725
HU 24063	A2	19821228	HU 1979-DU311	19790725
JP 55019300	A	19800209	JP 1979-95565	19790726
JP 63020801	B	19880430		
AU 7949687	A	19800501	AU 1979-49687	19790808
AU 526440	B2	19830113		
ES 490775	A1	19801201	ES 1980-490775	19800422
PRIORITY APPLN. INFO.:			NL 1978-7908	A 19780726
			GB 1979-25573	A 19790723

GI

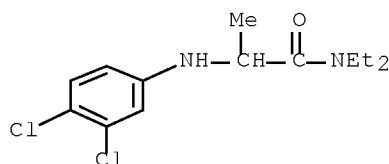


AB Algicidal compns. were prepared comprising a solid or liquid carrier and a diamine I (R = halo, alkyl, cycloalkyl, alkoxy, alkylthio, alkylsulfonyl, phenoxy, phenylthio, phenylalkyl; R¹ = H, alkyl, Ph, or CF₃; R² and R³ = H or alkyl; n = 2-6). E.g., I (R = 4-Cl, R¹ = H, R² = R³ = Et) [5427-35-0], prepared from N,N-diethylaminoethylchloride-HCl [869-24-9], killed >81% of Vaucheria, Cladophora, and Mougeotia at 0.4-2.0 mg/L after 2 wk.

IT 74474-39-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of)

RN 74474-39-8 ZCAPLUS

CN Propanamide, 2-[(3,4-dichlorophenyl)amino]-N,N-diethyl- (CA INDEX NAME)



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L58 ANSWER 79 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:215090 ZCAPLUS Full-text

DOCUMENT NUMBER: 92:215090

ORIGINAL REFERENCE NO.: 92:34831a,34834a

TITLE: Anti-depressant N-(3,4-dihalophenyl)-N-dimethylaminoalkylene amides

INVENTOR(S): Kane, Michael P.; Szmuszkowicz, Jacob

PATENT ASSIGNEE(S): Upjohn Co., USA

SOURCE: U.S., 10 pp. Cont.-in-Part of U.S. Ser. No. 934,239.
CODEN: USXXAM

DOCUMENT TYPE: Patent

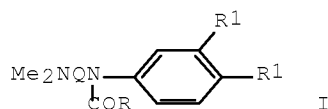
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4186208	A	19800129	US 1979-7127	19790129
US 4180522	A	19791225	US 1978-934239	19780816
PRIORITY APPLN. INFO.:			US 1976-746863	A1 19761202
			US 1977-838767	A1 19771003
			US 1978-934239	A2 19780816

GI



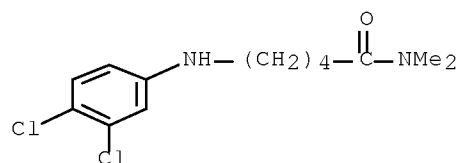
AB The title compds. I [Q = (CH₂)_n where n = 2-5, CH₂CHMeCH₂, CHMeCH₂, CH₂CHMe; R = Et, vinyl, cyclopropyl; R₁ = Br, Cl], useful as antidepressants (formulations and general dosage data reported), were prepared Thus, 3,4-Cl₂C₆H₃NH₂ with Me₂NCH₂CH₂Cl gave Me₂NCH₂CH₂NHC₆H₃Cl₂- 3,4 which with EtCOCl gave I [Q = (CH₂)₂, R = Et, R₁ = Cl].

IT 67447-04-5P 67447-07-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 67447-04-5 ZCAPLUS

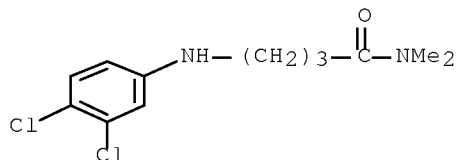
CN Pentanamide, 5-[(3,4-dichlorophenyl)amino]-N,N-dimethyl- (CA INDEX NAME)



RN 67447-07-8 ZCAPLUS

10/598508

CN Butanamide, 4-[(3,4-dichlorophenyl)amino]-N,N-dimethyl- (CA INDEX NAME)



L58 ANSWER 80 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:508204 ZCAPLUS Full-text

DOCUMENT NUMBER: 91:108204

ORIGINAL REFERENCE NO.: 91:17475a,17478a

TITLE: Synthesis of esters of N-substituted α -amino acids. 2. Preparation of esters of N-(3,4-dichlorophenyl)alanine in the presence of thionyl chloride

AUTHOR(S): Savin, V. P.; Sklyar, S. Ya.; Antipanova, V. E.; Sharnina, M. F.; Nayanova, V. A.

CORPORATE SOURCE: USSR

SOURCE: Doklady Neftekhimicheskoi Sektsii - Bashkirkoe Respublikanskoe Pravlenie Vsesoyuznogo Khimicheskogo Obshchestva imeni D. I. Mendeleeva (1976) 51-3
CODEN: DNSBAF

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB 3,4-Cl₂C₆H₃NHCHMeCO₂R (I; R = H) was esterified with EtOH in the presence of 8% SOCl₂ for 6 h with distillation of H₂O as the ternary azeotrope with EtOH and C₆H₆ to give 98.45% I (R = Et). I (R = Pr, Bu, C₅H₁₁) were prepared analogously in 38.19-52.33% yield using PhMe to remove H₂O.

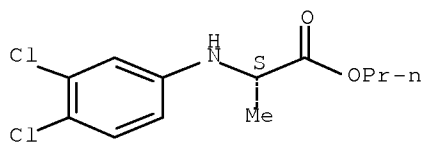
IT 71267-79-3P 71267-80-6P 71267-81-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71267-79-3 ZCAPLUS

CN L-Alanine, N-(3,4-dichlorophenyl)-, propyl ester (CA INDEX NAME)

Absolute stereochemistry.

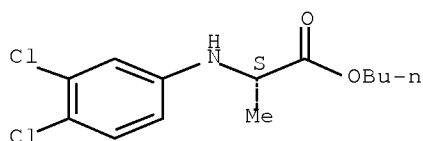


RN 71267-80-6 ZCAPLUS

CN L-Alanine, N-(3,4-dichlorophenyl)-, butyl ester (CA INDEX NAME)

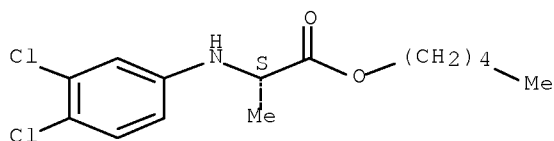
Absolute stereochemistry.

10/598508



RN 71267-81-7 ZCAPLUS
CN L-Alanine, N-(3,4-dichlorophenyl)-, pentyl ester (CA INDEX NAME)

Absolute stereochemistry.



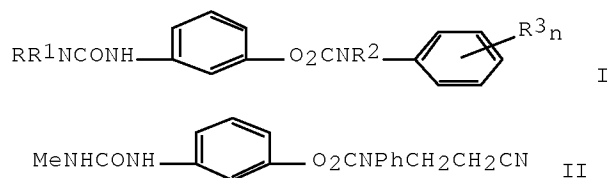
L58 ANSWER 81 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1979:186633 ZCAPLUS Full-text
DOCUMENT NUMBER: 90:186633
ORIGINAL REFERENCE NO.: 90:29645a,29648a
TITLE: Herbicidal carbanilic acid (3-ureidophenyl)esters
INVENTOR(S): Arndt, Friedrich; Nuesslein, Ludwig
PATENT ASSIGNEE(S): Schering A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 33 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2730325	A1	19790111	DE 1977-2730325	19770701
NL 7806766	A	19790103	NL 1978-6766	19780622
AU 7837539	A	19800103	AU 1978-37539	19780628
AU 518443	B2	19811001		
DK 7802948	A	19790102	DK 1978-2948	19780629
DD 135440	A5	19790509	DD 1978-206383	19780629
PL 110791	B1	19800731	PL 1978-208013	19780629
BE 868642	A1	19790102	BE 1978-188992	19780630
GB 2000500	A	19790110	GB 1978-28440	19780630
GB 2000500	B	19820224		
JP 54016450	A	19790207	JP 1978-79695	19780630
JP 56030343	B	19810714		
ES 471311	A1	19790901	ES 1978-471311	19780630
SU 797574	A3	19810115	SU 1978-2631495	19780630
CA 1100986	A1	19810512	CA 1978-306587	19780630
HU 24772	A2	19830428	HU 1978-SE650	19780630
CH 637634	A5	19830815	CH 1978-7188	19780630
HU 182600	B	19840228	HU 1978-SC650	19780630
FR 2395986	A1	19790126	FR 1978-19777	19780703

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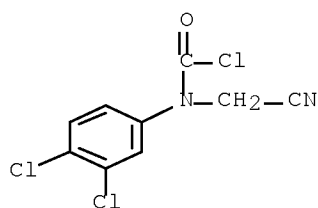
FR 2395986	B1	19840420		
CS 197326	B2	19800430	CS 1978-4415	19780703
US 4378318	A	19830329	US 1981-283667	19810715
PRIORITY APPLN. INFO.:			DE 1977-2730325	A 19770701
			US 1978-921106	A1 19780630
			US 1980-109687	A1 19800104

OTHER SOURCE(S): MARPAT 90:186633
GI



AB Sixty-nine ureidophenyl carbanilates I (R = C1-6 aliphatic chain or cyclic, saturated or unsatd. hydrocarbonyl; R1 = H, Me; R2 = cyanoalkyl, alkoxyalkyl; R3 = H, alkyl, alkoxy, alkylthio, halo; n = 1, 2), useful as pre- and post-emergence herbicides against Sinapis and Solanum (data tabulated) were prepared. Thus, a mixture of 85% KOH in MeOH and 3-HOC6H4NHCONHMe was evaporated in vacuo and the residue in MeCN refluxed with NCCH2CH2NPhCOCl 1 h to give 74% carbanilate II.

IT 55240-14-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(O-acylation of (hydroxyphenyl)urea derivative)
RN 55240-14-7 ZCAPLUS
CN Carbamic chloride, (cyanomethyl)(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)



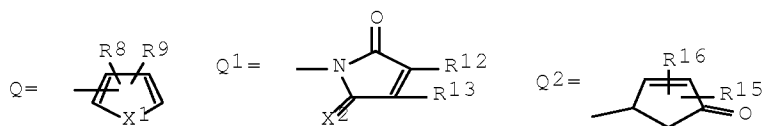
L58 ANSWER 82 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1979:122072 ZCAPLUS Full-text
DOCUMENT NUMBER: 90:122072
ORIGINAL REFERENCE NO.: 90:19348h,19349a,19350a
TITLE: Amino acid esters and thiol esters
INVENTOR(S): Henrick, Clive A.; Garcia, Barbara A.
PATENT ASSIGNEE(S): Zoecon Corp., USA
SOURCE: Ger. Offen., 89 pp.
CODEN: GWXXBX

10/598508

DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2812169	A1	19781005	DE 1978-2812169	19780320
DE 2812169	C2	19911017		
US 4243819	A	19810106	US 1978-878091	19780216
ZA 7801173	A	19790228	ZA 1978-1173	19780228
IN 148104	A1	19801018	IN 1978-CA264	19780313
ES 468013	A1	19781201	ES 1978-468013	19780318
BR 7801712	A	19781219	BR 1978-1712	19780320
BE 865114	A1	19780921	BE 1978-186111	19780321
PRIORITY APPLN. INFO.:			US 1977-779886	A 19770321
			US 1977-824947	A 19770815
			US 1978-878091	A 19780216

GI



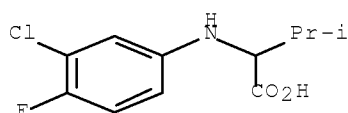
AB RR1NCR2R3COXR4 [R = cycloalkyl, cycloalkenyl, substituted Ph; R1 = H, alkyl, haloalkylcarbonyl, HCO; R2 = C2-5-alkyl, C2-5-alkenyl, C1-4-haloalkyl, C2-4-haloalkenyl, C3-4-cycloalkyl; R3 = H, F; X = O, S; R4 = CHR5R6 [R5 = H, CN, Me, CF3, C.tplbond.CH, CSNH2; R6 = substituted Ph, Q (R8 = H, alkyl; R9 = alkenyl, alkynyl, aralkyl; X1 = O, S)], CH2R10 [R10 = Q1 (R12R13 = alkylene, alkenylene; X2 = O, S), Q2 (R15 = H, alkyl, alkenyl, alkynyl, aralkyl; R16 = H, alkyl)], CH2CR17:CR18CH2R19 (R17 and R18 = H, Cl, F, Me; R17R18 = bond; R19 = Ph, OPh), CH(C.tplbond.CH)CR20:CHR21 (R20 = H, halo, Me, Et; R21 = allyl, propargyl, 3-butenyl, 3-butynyl, Ph, CH2Ph)] and their salts were prepared as pesticides. Thus, Me2CHCHBrCO2H was treated with SOCl2 to give the acid chloride, which was esterified with HOCH2C6H4OPh-m to give Me2CHCHBrCO2CH2C6H4OPh-m, which was aminated with PhNH2 to give PhNHCH(CHMe2)CO2CH2C6H4OPh-m. A great number of other N-substituted valine esters were also prepared. Pesticide activity data are given.

IT 69410-21-5 69410-70-4 69411-31-0
 69411-58-1 69411-82-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (esterification of, with phenoxybenzyl bromide)

RN 69410-21-5 ZCAPLUS

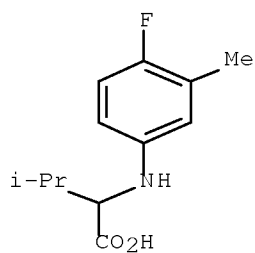
CN Valine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)



10/598508

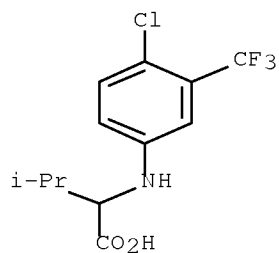
RN 69410-70-4 ZCAPLUS

CN Valine, N-(4-fluoro-3-methylphenyl)- (CA INDEX NAME)



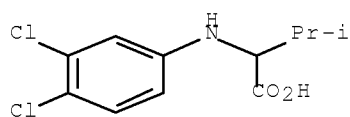
RN 69411-31-0 ZCAPLUS

CN Valine, N-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



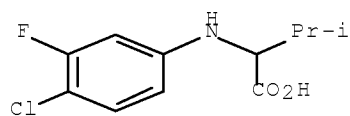
RN 69411-58-1 ZCAPLUS

CN Valine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)



RN 69411-82-1 ZCAPLUS

CN Valine, N-(4-chloro-3-fluorophenyl)- (CA INDEX NAME)



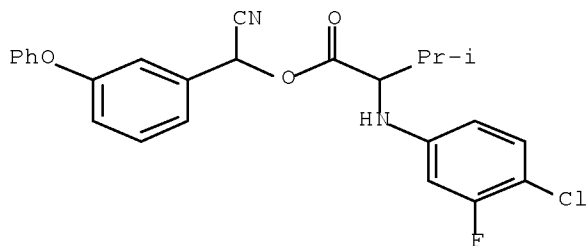
IT 69411-91-2P

10/598508

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and pesticide activity of)

RN 69411-91-2 ZCAPLUS

CN Valine, N-(4-chloro-3-fluorophenyl)-, cyano(3-phenoxyphenyl)methyl ester
(CA INDEX NAME)

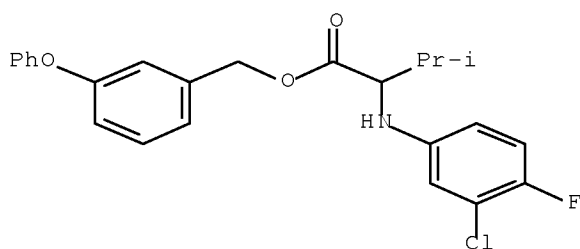


IT 69410-22-6P 69410-71-5P 69411-34-3P
69411-59-2P 69411-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

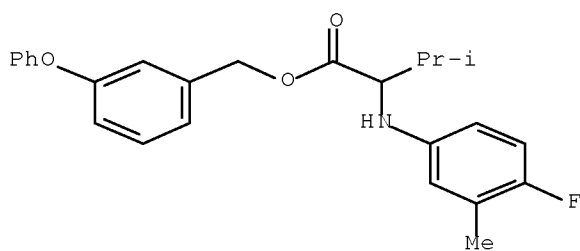
RN 69410-22-6 ZCAPLUS

CN Valine, N-(3-chloro-4-fluorophenyl)-, (3-phenoxyphenyl)methyl ester (CA
INDEX NAME)



RN 69410-71-5 ZCAPLUS

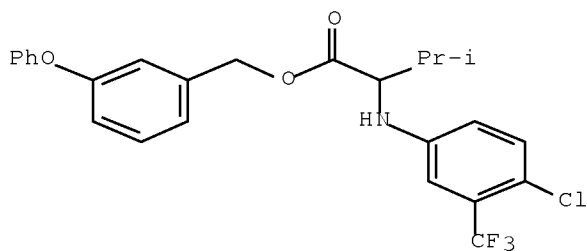
CN Valine, N-(4-fluoro-3-methylphenyl)-, (3-phenoxyphenyl)methyl ester (CA
INDEX NAME)



RN 69411-34-3 ZCAPLUS

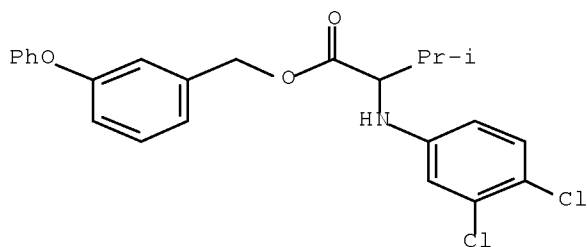
10/598508

CN Valine, N-[4-chloro-3-(trifluoromethyl)phenyl]-, (3-phenoxyphenyl)methyl ester (CA INDEX NAME)



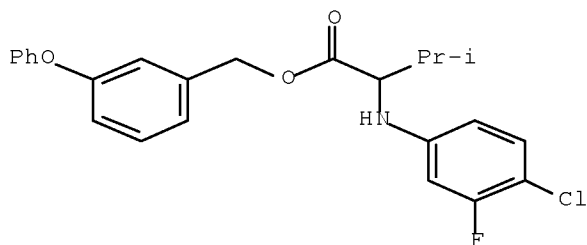
RN 69411-59-2 ZCAPLUS

CN Valine, N-(3,4-dichlorophenyl)-, (3-phenoxyphenyl)methyl ester (CA INDEX NAME)



RN 69411-87-6 ZCAPLUS

CN Valine, N-(4-chloro-3-fluorophenyl)-, (3-phenoxyphenyl)methyl ester (CA INDEX NAME)



L58 ANSWER 83 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:563572 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 89:163572

ORIGINAL REFERENCE NO.: 89:25357a,25360a

TITLE: Imidazole derivatives having fungicidal properties

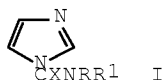
INVENTOR(S): Brookes, Robert Frederick; Godson, David Henry; Hams, Anthony Frederick; Weighton, David Michael; Wells,

10/598508

PATENT ASSIGNEE(S): Wilfred Hase
 SOURCE: Boots Co. Ltd., UK
 Pat. Specif. (Aust.), 61 pp.
 CODEN: ALXXAP
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AU 491880	B2	19780322	AU 1974-76526	19741217
AU 7476526	A	19760617		
GB 1469772	A	19770406	GB 1973-29535	19730621
JP 50031047	A	19750327	JP 1974-70743	19740620
JP 60010003	B	19850314		
DD 113164	A5	19750520	DD 1974-179314	19740620
CS 188185	B2	19790228	CS 1974-4365	19740620
FR 2234293	A1	19750117	FR 1974-21739	19740621
US 3991071	A	19761109	US 1974-532667	19741213
ZA 7408037	A	19760128	ZA 1974-8037	19741218
US 4154945	A	19790515	US 1978-879564	19780221
PRIORITY APPLN. INFO.:			GB 1973-29535	19730621
			US 1974-477734	A2 19740610
			US 1974-6532667	A3 19741213
			US 1975-720880	A3 19760907

GI



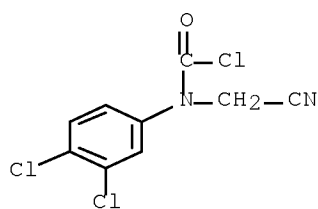
AB The fungicidal (no data) imidazoles I (R = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, Ph, phenylalkyl, phenylalkenyl, phenoxyalkyl, phenylthioalkyl; R1 = (un)substituted Ph, phenylalkyl, phenylalkenyl, phenoxyalkyl, phenylthioalkyl; X = O, S) (.apprx.300 compds.) were prepared Thus, 2-ClC6H4NHAc was treated with PrBr and the resulting 2-ClC6H4NHPr treated with Cl2CO to give 2-ClC6H4NPrCOCl, which was treated with imidazole to give I (R = 2-ClC6H4, R1 = Pr, X = O).

IT 55240-14-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction with imidazole)

RN 55240-14-7 ZCAPLUS

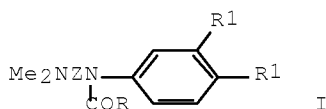
CN Carbamic chloride, (cyanomethyl)(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)

10/598508



L58 ANSWER 84 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1978:508608 ZCAPLUS Full-text
 DOCUMENT NUMBER: 89:108608
 ORIGINAL REFERENCE NO.: 89:16701a,16704a
 TITLE: Aminoamides
 INVENTOR(S): Kane, Michael Paul; Szmuszkowicz, Jacob
 PATENT ASSIGNEE(S): Upjohn Co., USA
 SOURCE: Ger. Offen., 61 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2751905	A1	19780608	DE 1977-2751905	19771121
DE 2751905	C2	19870611		
AU 7730376	A	19790517	AU 1977-30376	19771107
AU 509345	B2	19800508		
GB 1542749	A	19790321	GB 1977-46751	19771110
CH 636596	A5	19830615	CH 1977-14293	19771122
SE 7713442	A	19780603	SE 1977-13442	19771128
SE 441445	B	19851007		
SE 441445	C	19860403		
NL 7713204	A	19780606	NL 1977-13204	19771130
FR 2372796	A1	19780630	FR 1977-36186	19771130
FR 2372796	B1	19800822		
BE 861455	A1	19780602	BE 1977-183134	19771202
JP 53071024	A	19780624	JP 1977-144917	19771202
JP 62020182	B	19870506		
SE 8304187	A	19830728	SE 1983-4187	19830728
PRIORITY APPLN. INFO.:			US 1976-746863	A 19761202
OTHER SOURCE(S):	MARPAT	89:108608		
GI				



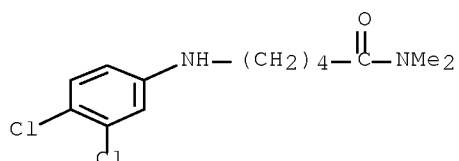
10/598508

AB Seven acylanilines I [R = Et, cyclopropyl, vinyl; R1 = Cl, Br; Z = (CH2)n (n = 2-5), CHMeCH2, CH2CHMe, CH2CHMeCH2] and their resp. pharmacol. acceptable salts, useful as antidepressants at 0.05-1 mg/kg in humans, were prepared by 2 methods. Thus, 3,4-Cl2C6H3NH2 was heated 72 h at 100° with ClCH2CH2NMe2 and the product 3,4-Cl2C6H3NHCH2CH2NMe2 acylated with EtCOCl in CH2Cl2 containing NEt3 to give I (R = Et, R1 = Cl, Z = CH2CH2), characterized as the maleate. Cl(CH2)4COCl was aminated with Me2NH and the product Cl(CH2)4CONMe2 successively treated with 3,4-Cl2C6H3NH2, the 3,4-Cl2C6H3NH(CH2)4CONMe2 reduced and 3,4-Cl2C6H3NH(CH2)5NMe2 acylated with (EtCO)2O to give I [R = Me, R1 = Cl, Z = (CH2)5], characterized as the oxalate.

IT 67447-04-5P 67447-07-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of)

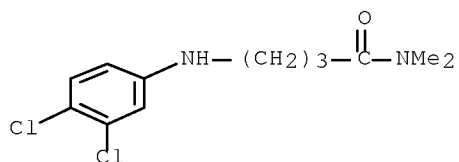
RN 67447-04-5 ZCAPLUS

CN Pentanamide, 5-[(3,4-dichlorophenyl)amino]-N,N-dimethyl- (CA INDEX NAME)



RN 67447-07-8 ZCAPLUS

CN Butanamide, 4-[(3,4-dichlorophenyl)amino]-N,N-dimethyl- (CA INDEX NAME)



L58 ANSWER 85 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:22917 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 88:22917

ORIGINAL REFERENCE NO.: 88:3685a,3688a

TITLE: Acetohydroxamic acids

INVENTOR(S): Lafon, Louis

PATENT ASSIGNEE(S): Laboratoire L. Lafon S. A., Fr.

SOURCE: Ger. Offen., 105 pp.
 CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2711451	A1	19771006	DE 1977-2711451	19770316
DE 2711451	C2	19900510		
GB 1574822	A	19800910	GB 1976-11710	19760323
FR 2345430	A1	19771021	FR 1977-6997	19770309
FR 2345430	B1	19820723		
ZA 7701584	A	19780726	ZA 1977-1584	19770316
AU 7723344	A	19780921	AU 1977-23344	19770317
AU 516473	B2	19810604		
US 4122186	A	19781024	US 1977-778543	19770317
FI 7700859	A	19770924	FI 1977-859	19770318
FI 62821	B	19821130		
FI 62821	C	19830310		
AT 7701930	A	19790915	AT 1977-1930	19770321
AT 356078	B	19800410		
CH 620894	A5	19801231	CH 1977-3479	19770321
IL 51705	A	19820930	IL 1977-51705	19770321
BE 852738	A1	19770922	BE 1977-175998	19770322
DK 7701266	A	19770924	DK 1977-1266	19770322
DK 171197	B1	19960722		
SE 7703263	A	19770924	SE 1977-3263	19770322
SE 432420	B	19840402		
SE 432420	C	19840712		
NO 7701006	A	19770926	NO 1977-1006	19770322
NO 144420	B	19810518		
NO 144420	C	19810826		
HU 172677	B	19771128	HU 1977-LA912	19770322
CS 200511	B2	19800915	CS 1977-1904	19770322
NL 7703168	A	19770927	NL 1977-3168	19770323
NL 188801	B	19920506		
NL 188801	C	19921001		
JP 52144601	A	19771202	JP 1977-32011	19770323
JP 62008424	B	19870223		
DD 129645	A5	19780201	DD 1977-198023	19770323
SU 689617	A3	19790930	SU 1977-2465454	19770323
PL 113772	B1	19801231	PL 1977-198229	19770519
BE 863947	A4	19780529	BE 1978-185158	19780214
US 4151300	A	19790424	US 1978-930927	19780804
US 4152458	A	19790501	US 1978-930926	19780804
US 4183951	A	19800115	US 1978-930925	19780804
US 4209523	A	19800624	US 1978-930924	19780804
US 4209524	A	19800624	US 1978-930928	19780804
AT 7808399	A	19800215	AT 1978-8399	19781124
AT 358556	B	19800925		
AT 7808398	A	19800915	AT 1978-8398	19781124
AT 361932	B	19810410		
AT 7808400	A	19801115	AT 1978-8400	19781124
AT 362793	B	19810610		
US 4225617	A	19800930	US 1979-69254	19790824
US 4325964	A	19820420	US 1979-107609	19791227
FR 2453148	A1	19801031	FR 1980-5644	19800313
FR 2453148	B1	19831202		
FR 2453133	A1	19801031	FR 1980-5645	19800313
FR 2453133	B1	19840406		
FR 2453158	A1	19801031	FR 1980-5646	19800313
FR 2453158	B1	19820806		
AT 8005014	A	19830815	AT 1980-5014	19801009
AT 374191	B	19840326		
NO 8003336	A	19770926	NO 1980-3336	19801106
NO 146431	B	19820621		
NO 146431	C	19820929		

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NO 8003337	A	19770926	NO 1980-3337	19801106
NO 152972	B	19850916		
NO 152972	C	19851227		
NO 8003338	A	19770926	NO 1980-3338	19801106
NO 145881	B	19820308		
NO 145881	C	19820616		
FI 8201213	A	19820406	FI 1982-1213	19820406
FI 65236	B	19831230		
FI 65236	C	19840410		
FI 8201214	A	19820406	FI 1982-1214	19820406
FI 69624	B	19851129		
FI 69624	C	19860310		
FI 8201215	A	19820406	FI 1982-1215	19820406
FI 71313	B	19860909		
FI 71313	C	19861219		
SE 8302171	A	19830419	SE 1983-2171	19830419
SE 452155	B	19871116		
SE 452155	C	19880225		
SE 8302172	A	19830419	SE 1983-2172	19830419
SE 458605	B	19890417		
SE 458605	C	19890810		
SE 8302173	A	19830419	SE 1983-2173	19830419
SE 456992	B	19881121		
SE 456992	C	19890316		

PRIORITY APPLN. INFO.:

GB 1976-11710	A	19760323
GB 1977-6298	A	19770215
US 1977-778543	A3	19770317
FI 1977-859	A	19770318
AT 1977-1930	A	19770321
GB 1977-16705	A	19770421
US 1978-877963	A1	19780215
US 1978-930925	A3	19780804

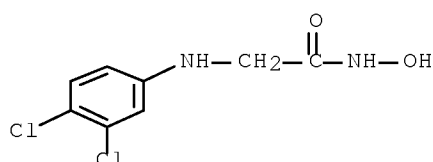
AB Psychotropic RCONHOH (R = e.g. C₄H₉, 5,5-diphenylhydantoinylmethyl, CH₂CONPh₂, CH₂NHCOCHPh₂, CH₂SOCH₂C₆H₄Cl-4, phenothiazinylethyl, 1-phenyl-2-benzimidazolylmethyl, CH₂NHC₆H₃Cl₂-3,4, CH₂NHCONHC₆H₄Cl-4) (38 compds.) were prepared. Thus, Bu₃CCO₂H was chlorinated and treated with NH₂OH.HCl to give 48% Bu₃C₂CONHOH, which had tranquilizing activity in mice. Ph₂NCOCH₂CONHOH, at 100 mg/kg in 2 doses 2 h apart in rats, also lowered arterial blood pressure 10% and decreased heart frequency 8%.

IT 14108-53-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and psychotropic activity of)

RN 14108-53-3 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-hydroxy- (CA INDEX NAME)

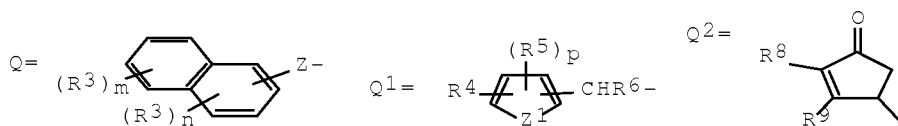


10/598508

DOCUMENT NUMBER: 88:22601
 ORIGINAL REFERENCE NO.: 88:3625a,3628a
 TITLE: Acetic acid derivatives
 INVENTOR(S): Fujita, Sumio; Nakajima, Minoru; Fujita, Toshio
 PATENT ASSIGNEE(S): Dainippon Jochugiku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52091833	A	19770802	JP 1976-7034	19760124
JP 62037031	B	19870810		

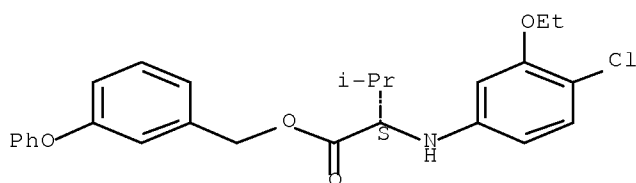
PRIORITY APPLN. INFO.: JP 1976-7034 A 19760124
 GI



AB Thirty seven title derivs. $RR_1CHCO_2R_2$ I [R = (R³)mC₆H₄-mNH (R³ = alkyl, alkoxy, halo; m = 1-4), Q (n = 1-3, Z = O, S, a bond); R₁ = alkyl, alkenyl, alkoxy, haloalkyl, etc.; R₂ = Q¹ (R⁴ = H, aryl, etc.; R⁵ = H, Me, F₃C, halo; p = 1-2; R⁴ and R⁵ may be bound to form a ring; R⁶ = H, ethynyl, cyano; Z¹ = O, X, CH:CH), R⁷CH₂ (R⁷ = phthalimido, etc.); Q² (R⁸ = H₂C:CH, etc.; R⁹ = H, Me); R¹⁰CH₂CR¹¹:CHCH₂ (R¹⁰ = Ph, etc.; R¹¹ = Me, halo)] were prepared by reaction of RR₁CHCO₂H or their reactive derivs. with R₂OH. I are useful as insecticides; the data were given against *Musca domestica*, *Culex pipiens pallens*, *Prodenia litura*, *Myrus persicae*, and *Delphacodes striatella*. Thus, a sealed mixture of 4.8 g α-isopropyl-(p-methoxyanilino)acetic acid chloride, 4.2 g 3-PhOC₆H₄CH₂OH, and 3 mL pyridine in C₆H₆ was allowed to stand overnight at room temperature to give 7.2 g I (R = 4-MeOC₆H₄NH, R₁ = Me₂CH, R₂ = 3-PhOC₆H₄CH₂).

IT 64971-84-2F
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and insecticidal activity of)
 RN 64971-84-2 ZCAPLUS
 CN L-Valine, N-(4-chloro-3-ethoxyphenyl)-, (3-phenoxyphenyl)methyl ester (CA INDEX NAME)

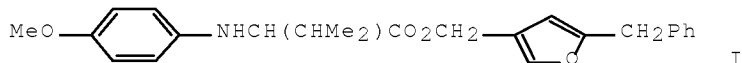
Absolute stereochemistry.



L58 ANSWER 87 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1978:17338 ZCAPLUS Full-text
 DOCUMENT NUMBER: 88:17338
 ORIGINAL REFERENCE NO.: 88:2751a,2754a
 TITLE: Phenoxbenzyl alkylacetate insecticides
 INVENTOR(S): Katsuta, Sumio
 PATENT ASSIGNEE(S): Dainippon Jochugiku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52082724	A	19770711	JP 1975-156335	19751229
JP 57048522	B	19821016		

PRIORITY APPLN. INFO.: JP 1975-156335 A 19751229
 GI

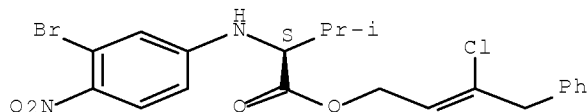


AB Esters of (phenylamino)alkylacetic acids are wide-spectrum insecticides. Thus, 5'-benzyl-3'-furylmethyl α -isopropyl-(p-methoxyanilino)acetate (I) [64823-66-1] was synthesized from α -isopropyl-(p-methoxyanilino)acetic acid chloride [64823-70-7] and 5-benzyl-3-furylmethanol [20416-09-5]. A solution of I (1:200 dilution) was applied to a Japanese white radish field infested with *Myzus persicae* at 100 L/tan (0.245 acre). The *M. persicae* population decreased to <10% in 2 days.

IT 64823-56-9P 64823-65-0P
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and insecticidal activity of)
 RN 64823-56-9 ZCAPLUS
 CN L-Valine, N-(3-bromo-4-nitrophenyl)-, 3-chloro-4-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

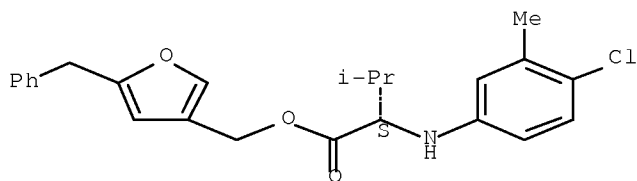
Absolute stereochemistry.
 Double bond geometry unknown.

10/598508



RN 64823-65-0 ZCAPLUS
 CN L-Valine, N-(4-chloro-3-methylphenyl)-, [5-(phenylmethyl)-3-furanyl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 88 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1978:6708 ZCAPLUS Full-text
 DOCUMENT NUMBER: 88:6708
 ORIGINAL REFERENCE NO.: 88:1133a,1136a
 TITLE: Anilinoacetates
 INVENTOR(S): Katsuta, Sumio
 PATENT ASSIGNEE(S): Dainippon Jochugiku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52100431	A	19770823	JP 1976-16179	19760217
JP 58052987	B	19831126		
PRIORITY APPLN. INFO.: GI			JP 1976-16179	A 19760217



AB Forty-four anilinoacetates [I, Rn = H, 4-Cl, -Me, -MeO, 3-Cl, 3-MeCO, 3,4-(methylenedioxy), 2,4-(MeO)2, etc.; R1 = CHMe2, CCl:CH2, Et, CHCl2, etc.; R2 = 5-benzyl-3-furylmethoxy, OCH2C6H4OPh-m, dimethylmaleimidomethoxy, etc.] were

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prepared and 42 of them were evaluated for their insecticidal activity. Thus, 5.3 g I (Rn = 4-MeO, R1 = CHMe2, R2 = Cl) in benzene was treated with 3.7 g 5-benzyl-3-furanmethanol in the presence of pyridine to give 8.2 g I (Rn = 4-MeO, R1 = CHMe2, R2 = 5-benzyl-3-furylmethoxy).

IT 64823-56-9F 64823-65-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

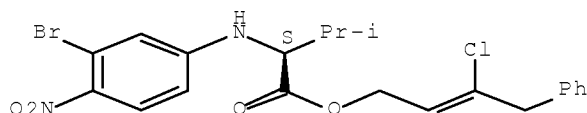
(preparation and insecticidal activity of)

RN 64823-56-9 ZCAPLUS

CN L-Valine, N-(3-bromo-4-nitrophenyl)-, 3-chloro-4-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

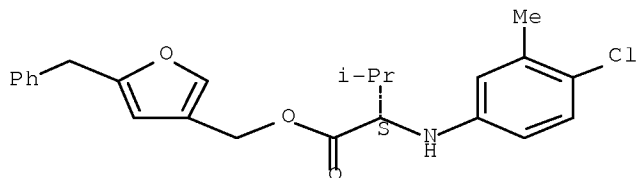
Double bond geometry unknown.



RN 64823-65-0 ZCAPLUS

CN L-Valine, N-(4-chloro-3-methylphenyl)-, [5-(phenylmethyl)-3-furanyl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 89 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:567761 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 87:167761

ORIGINAL REFERENCE NO.: 87:26503a,26506a

TITLE: Substituted phenylamidines

INVENTOR(S): Lafon, Louis

PATENT ASSIGNEE(S): Laboratoire L. Lafon, Fr.

SOURCE: Ger. Offen., 44 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2702119	A1	19770728	DE 1977-2702119	19770120
DE 2702119	C2	19860710		

10/598508

GB 1538097	A	19790117	GB 1976-2895	19760126
CH 620901	A5	19801231	CH 1977-273	19770111
FR 2338927	A1	19770819	FR 1977-1595	19770120
FR 2338927	B1	19801010		
CA 1074797	A1	19800401	CA 1977-270277	19770124
BE 850723	A1	19770516	BE 1977-174356	19770125
DK 7700302	A	19770727	DK 1977-302	19770125
SE 7700777	A	19770727	SE 1977-777	19770125
SE 440501	B	19850805		
SE 440501	C	19851114		
US 4146647	A	19790327	US 1977-762774	19770125
NL 7700806	A	19770728	NL 1977-806	19770126
NL 188573	B	19920302		
NL 188573	C	19920803		
JP 52105131	A	19770903	JP 1977-7602	19770126
JP 59053895	B	19841227		

PRIORITY APPLN. INFO.:

GB 1976-2895

A 19760126

OTHER SOURCE(S):

MARPAT 87:167761

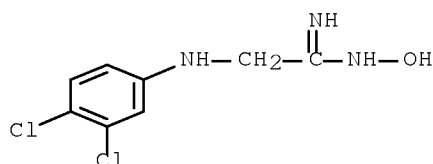
AB RR1C6H3ZC(NHR2):NR3 (I; R = Cl, Me, OMe, OEt; R1 = H, Cl, Me, OMe, OEt; R2 = OH, CH2CO2Et; R3 = H; R2R3 = CH2CH2, N:N, etc.; Z = CHOH, CH2, NHCOCH2, NH, CH2S, etc.) were prepared. Thus, an aqueous solution of HCl and KCN was added to a mixture of 3,4-Cl2C6H3CHO and aqueous NaHSO3 to give 3,4-Cl2C6H3CH(OH)CN, which was treated with HCl/EtOH to give 3,4-Cl2C6H3CH(OH)C(OEt):NH.HCl. Reaction of the imidic ester with H2NCH2CO2Et gave I (RR1 = 3,4-Cl2; R2 = CH2CO2Et, R3 = H, Z = CHOH) (II). About 15 I were prepared, useful as antihypertensives and antidepressants, e.g., II at 100 mg/kg gave 20% lowering of blood pressure in the mouse.

IT 64204-49-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 64204-49-5 ZCAPLUS

CN Ethanimidamide, 2-[(3,4-dichlorophenyl)amino]-N-hydroxy-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L58 ANSWER 90 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:467990 ZCAPLUS Full-text

DOCUMENT NUMBER: 87:67990

ORIGINAL REFERENCE NO.: 87:10809a,10812a

TITLE: Aniline derivatives with herbicidal action

INVENTOR(S): Scott, Richard Mark; Armitage, Geoffrey David

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.,
Neth.

SOURCE: Ger. Offen., 15 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

10/598508

LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2650434	A1	19770518	DE 1976-2650434	19761103
DE 2650434	C2	19890126		
GB 1563201	A	19800319	GB 1975-45914	19751105
CA 1110268	A1	19811006	CA 1976-263684	19761019
FR 2330671	A1	19770603	FR 1976-32780	19761029
FR 2330671	B1	19790608		
US 4267355	A	19810512	US 1976-737313	19761101
JP 52059120	A	19770516	JP 1976-131329	19761102
JP 61013462	B	19860414		
BE 847891	A2	19770503	BE 1976-1007736	19761103
DK 7604979	A	19770506	DK 1976-4979	19761103
DK 149194	B	19860310		
DK 149194	C	19860804		
NL 7612166	A	19770509	NL 1976-12166	19761103
NL 187266	B	19910301		
NL 187266	C	19910801		
BR 7607351	A	19770920	BR 1976-7351	19761103
IL 50837	A	19790725	IL 1976-50837	19761103
AU 507720	B2	19800228	AU 1976-19277	19761103
AU 7619277	A	19780511		
CH 623803	A5	19810630	CH 1976-13865	19761103
SU 932983	A3	19820530	SU 1976-2417802	19761103
			GB 1975-45914	A 19751105

PRIORITY APPLN. INFO.:

AB (R)-3,4-ClRC₆H₃NR₁CHMeCO₂R₂ (I; R = F, Cl; R₁ = H, Bz; R₂ = Me, Et, Me₂CH, etc.) were prepared by the reaction of (S)-R₃OCHMeCO₂R₂ (R₂ as above, R₃ = Bz, MeSO₂) with 3,4-ClRC₆H₃NH₂, then with BzCl. I are useful as herbicides (no data).

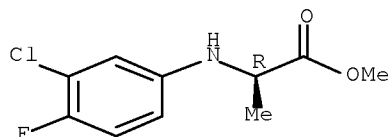
IT 62766-88-5P 62836-62-8P 62836-63-9P
 62840-19-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 62766-88-5 ZCAPLUS

CN D-Alanine, N-(3-chloro-4-fluorophenyl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

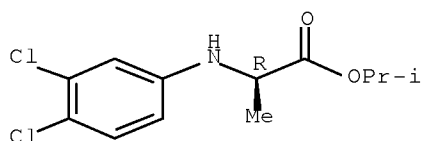


RN 62836-62-8 ZCAPLUS

CN D-Alanine, N-(3,4-dichlorophenyl)-, 1-methylethyl ester (CA INDEX NAME)

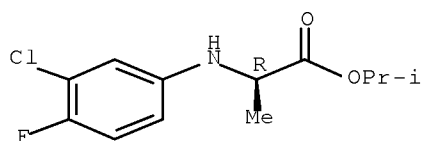
Absolute stereochemistry.

10/598508



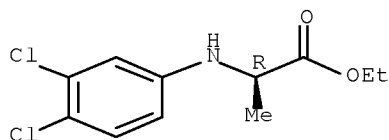
RN 62836-63-9 ZCAPLUS
CN D-Alanine, N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 62840-19-1 ZCAPLUS
CN D-Alanine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

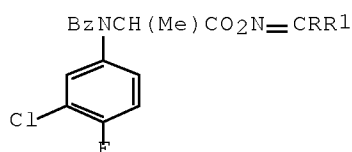


L58 ANSWER 91 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:453586 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 87:53586
ORIGINAL REFERENCE NO.: 87:8523a,8526a
TITLE: Herbicidal N,N-disubstituted alanine derivatives
INVENTOR(S): Haddock, Ernest; Hopwood, William J.
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.,
Neth.
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2628901	A1	19770120	DE 1976-2628901	19760628
DE 2628901	C2	19860109		
CA 1088089	A1	19801021	CA 1976-254661	19760611

10/598508

NL 7607051	A	19770103	NL 1976-7051	19760628
NL 183398	B	19880516		
NL 183398	C	19881017		
JP 52005726	A	19770117	JP 1976-75667	19760628
JP 60058745	B	19851221		
FR 2316221	A1	19770128	FR 1976-19585	19760628
FR 2316221	B1	19790406		
ZA 7603841	A	19770525	ZA 1976-3841	19760628
AU 510514	B2	19800703	AU 1976-15368	19760628
SU 803844	A3	19810207	SU 1976-2376123	19760628
CH 623202	A5	19810529	CH 1976-8264	19760628
PRIORITY APPLN. INFO.:			GB 1975-27482	A 19750630
GI				



I

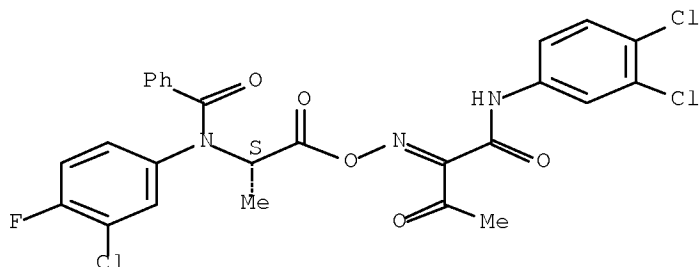
AB Alanine oxime esters I (R = Ac, R1 = COPr, CONHPh, CONHMe, CONEt2, CONHC6H3Cl2-3,4; R = Me, R1 = COEt), useful as herbicides, were prepared by esterifying N-benzoyl-N-(3-chloro-4-fluorophenyl)alanine (II) with HON:CRR1. Thus, II was condensed with HON:CMCOEt in CH2Cl2 by dicyclohexylcarbodiimide to give 21% I (R = Me, R1 = COEt). I were tested as preemergence and postemergence herbicides in 9 plants.

IT 63236-45-3P
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and herbicidal activity of)

RN 63236-45-3 ZCAPLUS

CN Benzamide, N-(3-chloro-4-fluorophenyl)-N-[2-[[[1-[[[3,4-dichlorophenyl]amino]carbonyl]-2-oxopropylidene]amino]oxy]-1-methyl-2-oxoethyl]-, (S)- (9CI) (CA INDEX NAME)

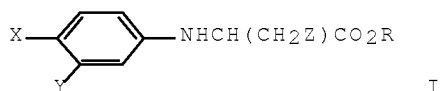
Absolute stereochemistry.
 Double bond geometry unknown.



10/598508

ACCESSION NUMBER: 1977:417307 ZCAPLUS Full-text
 DOCUMENT NUMBER: 87:17307
 ORIGINAL REFERENCE NO.: 87:2713a,2716a
 TITLE: Herbicidal composition containing N-substituted
 alanine derivatives
 INVENTOR(S): Haddock, Ernest; Raven, Clive Alan; Sampson, Alan John
 PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.,
 Neth.
 SOURCE: Ger. Offen., 25 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2633729	A1	19770217	DE 1976-2633729	19760727
DE 2633729	C2	19960926		
GB 1547758	A	19790627	GB 1975-31691	19750729
CA 1161657	A1	19840207	CA 1976-256530	19760707
NL 7608288	A	19770201	NL 1976-8288	19760727
FR 2319299	A1	19770225	FR 1976-22839	19760727
FR 2319299	B1	19800328		
AU 509210	B2	19800501	AU 1976-16277	19760727
CH 622674	A5	19810430	CH 1976-9596	19760727
JP 60051442	B	19851114	JP 1976-88753	19760727
JP 60016957	A	19850128	JP 1984-95764	19840515
JP 62061583	B	19871222		
PRIORITY APPLN. INFO.:			GB 1975-31691	A 19750729
GI				



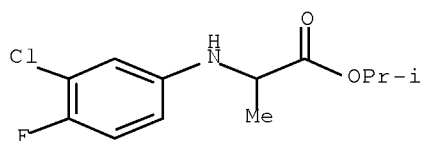
AB The title compds. I (X = Cl, F; Y = H, Cl, F; Z = H, alkoxy; R = H or Cl-4 alkyl) and mixts. of their optical isomers are herbicides. Thus, N-(3-chloro-4-fluorophenyl)alanine [62766-92-1] showed high toxicity to mustard and low toxicity to barley.

IT 52756-24-8 62766-87-4 62766-88-5
 62766-89-6 62766-91-0 62766-92-1
 62766-93-2 62836-62-8 62836-63-9
 62840-19-1 62840-20-4
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
 (herbicide)

RN 52756-24-8 ZCAPLUS

CN Alanine, N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester (CA INDEX NAME)

10/598508



RN 62766-87-4 ZCAPLUS

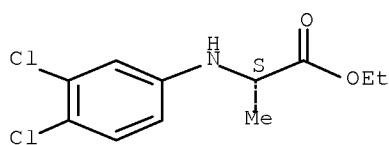
CN L-Alanine, N-benzoyl-N-(3,4-dichlorophenyl)-, ethyl ester, mixt. with
N-(3,4-dichlorophenyl)-L-alanine ethyl ester (9CI) (CA INDEX NAME)

CM 1

CRN 33878-52-3

CMF C11 H13 Cl2 N O2

Absolute stereochemistry.

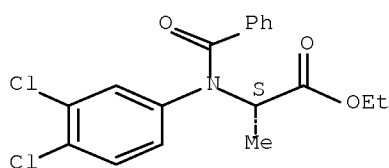


CM 2

CRN 33878-50-1

CMF C18 H17 Cl2 N O3

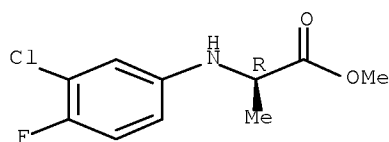
Absolute stereochemistry.



RN 62766-88-5 ZCAPLUS

CN D-Alanine, N-(3-chloro-4-fluorophenyl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



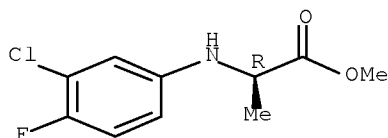
10/598508

RN 62766-89-6 ZCAPLUS
CN D-Alanine, N-(3-chloro-4-fluorophenyl)-, methyl ester, mixt. with
N-benzoyl-N-(3-chloro-4-fluorophenyl)-L-alanine methyl ester (9CI) (CA
INDEX NAME)

CM 1

CRN 62766-88-5
CMF C10 H11 Cl F N O2

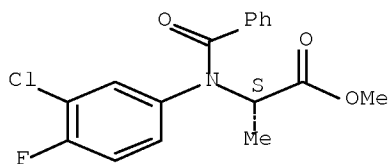
Absolute stereochemistry.



CM 2

CRN 57973-66-7
CMF C17 H15 Cl F N O3

Absolute stereochemistry.



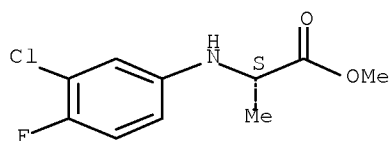
RN 62766-91-0 ZCAPLUS
CN L-Alanine, N-benzoyl-N-(3-chloro-4-fluorophenyl)-, methyl ester, mixt.
with N-(3-chloro-4-fluorophenyl)-L-alanine methyl ester (9CI) (CA INDEX
NAME)

CM 1

CRN 62766-90-9
CMF C10 H11 Cl F N O2

Absolute stereochemistry.

10/598508

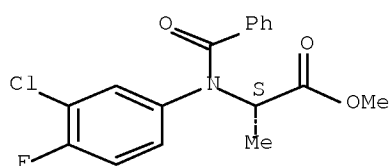


CM 2

CRN 57973-66-7

CMF C17 H15 Cl F N O3

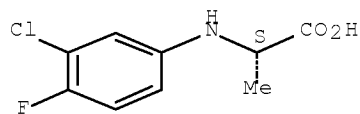
Absolute stereochemistry.



RN 62766-92-1 ZCAPLUS

CN L-Alanine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 62766-93-2 ZCAPLUS

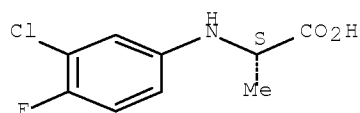
CN L-Alanine, N-benzoyl-N-(3-chloro-4-fluorophenyl)-, methyl ester, mixt.
with N-(3-chloro-4-fluorophenyl)-L-alanine (9CI) (CA INDEX NAME)

CM 1

CRN 62766-92-1

CMF C9 H9 Cl F N O2

Absolute stereochemistry.



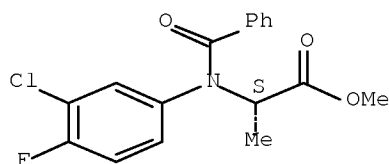
10/598508

CM 2

CRN 57973-66-7

CMF C17 H15 Cl F N O3

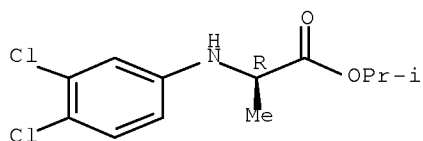
Absolute stereochemistry.



RN 62836-62-8 ZCAPLUS

CN D-Alanine, N-(3,4-dichlorophenyl)-, 1-methylethyl ester (CA INDEX NAME)

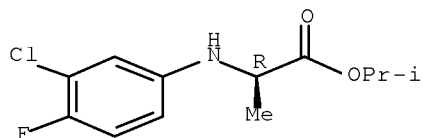
Absolute stereochemistry.



RN 62836-63-9 ZCAPLUS

CN D-Alanine, N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester (CA INDEX NAME)

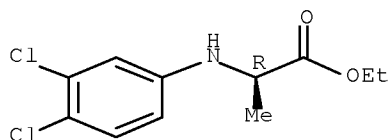
Absolute stereochemistry.



RN 62840-19-1 ZCAPLUS

CN D-Alanine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



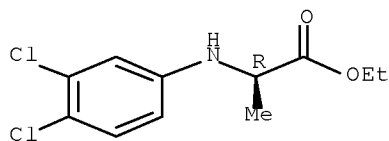
10/598508

RN 62840-20-4 ZCAPLUS
CN D-Alanine, N-(3,4-dichlorophenyl)-, ethyl ester, mixt. with
N-benzoyl-N-(3-chloro-4-fluorophenyl)-L-alanine methyl ester (9CI) (CA
INDEX NAME)

CM 1

CRN 62840-19-1
CMF C11 H13 Cl2 N O2

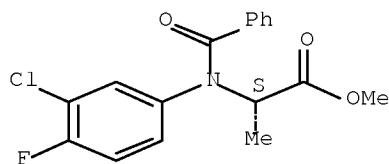
Absolute stereochemistry.



CM 2

CRN 57973-66-7
CMF C17 H15 Cl F N O3

Absolute stereochemistry.

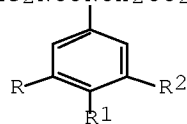


L58 ANSWER 93 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:190461 ZCAPLUS Full-text
DOCUMENT NUMBER: 86:190461
ORIGINAL REFERENCE NO.: 86:29892h,29893a
TITLE: N-Carbamoyl-N-phenylamino acid derivatives with
herbicides properties
INVENTOR(S): Hashimoto, Shunichi; Kameda, Nobuyuki; Fujinami, Akira
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Ger. Offen., 39 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

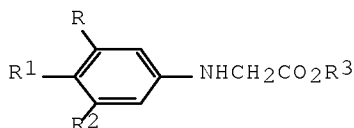
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2624094	A1	19761202	DE 1976-2624094	19760528
JP 51139626	A	19761202	JP 1975-64881	19750529
JP 52012248	B	19770406		
FR 2312491	A1	19761224	FR 1976-16011	19760526
NL 7605866	A	19761201	NL 1976-5866	19760531
PRIORITY APPLN. INFO.:			JP 1975-64881	A 19750529

GI



I



II

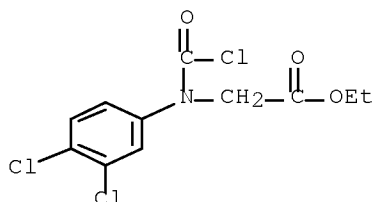
AB Twenty-seven N-(dimethylcarbamyl)-N-phenyl glycines I [R = H, Me, Et, MeO, CF₃, Cl; R₁ = H, Me, Pr, Cl, Br, MeO, BuO, Me(CH₂)₅; R₂ = H, Cl; R₃ = H, Me, Et, Pr, CHMe₂, Bu, CH₂CHMe₂, (CH₂)₄Me, (CH₂)₅Me, cyclohexyl] and 16 other N-carbamyl-N-phenyl amino acid derivs. e.g., Me₃NCONPhCH₂CH₂CH₂CO₂Et, Pr₂NCONPhCH₂CO₂Et were prepared as herbicides. Thus, I [R = H, Me, Et, MeO, R₁ = R₂ = H, R₃ = Et; R = R₂ = H, R₁ = Me(CH₂)₅, MeO, BuO, Cl, R₃ = Et; R = R₁ = H, Me, R₂ = H, R₃ = Et, Pr] were prepared in 64-88% yields by acylating the appropriate N-phenylglycine derivative II with Me₂NCOCl. 3,4-Cl₂C₆H₃NHCH₂CO₂Et was treated with COCl₂ in the presence of pyridine to give 3,4-Cl₂C₆H₃N(COCl)CH₂CO₂Et which was treated with Me₂NH to give 89% I (R = R₁ = Cl, R₂ = H, R₃ = Et). Twenty-seven other N-carbamyl-N-phenyl amino acids were also prepared by treating their N-(chlorocarbonyl) derivs. with amines. I (R = R₁ = H, Cl, R₂ = H, R₃ = Et; R = Et, R₁ = R₂ = H, R₃ = Et) and Me₂NCONPhCHMeCO₂Et were saponified to their corresponding free acids in 63-71% yields. Herbicidal activities are given for 42 synthetic N-carbamyl-N-phenyl amino acids.

IT 62750-16-7F

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with amines)

RN 62750-16-7 ZCAPLUS

CN Glycine, N-(chlorocarbonyl)-N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)



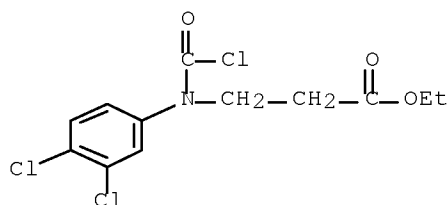
IT 62750-30-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethylamine)

10/598508

RN 62750-30-5 ZCAPLUS

CN β -Alanine, N-(chlorocarbonyl)-N-(3,4-dichlorophenyl)-, ethyl ester
(CA INDEX NAME)



L58 ANSWER 94 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1976:505425 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 85:105425

ORIGINAL REFERENCE NO.: 85:16889a,16892a

TITLE: Methyl or isopropyl N-(3-chloro-4-fluorophenyl)-N-benzoyl-2-aminopropionate-containing composition with selective herbicidal activity

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.,
Neth.

SOURCE: Austrian, 6 pp.

CODEN: AUXXAK

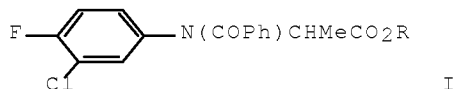
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 329916	B	19760610	AT 1973-8466	19731004
AT 7308466	A	19750815		
PRIORITY APPLN. INFO.: GI			AT 1973-8466	A 19731004



AB The title compds. I (R = Me or iso-Pr) are selective herbicides for control of wild oat (*Avena fatua*) in cereals. Thus, in pot expts., Me N-benzoyl-N-(3-chloro-4-fluorophenyl)-2-aminopropionate [52756-25-9] showed high toxicity to wild oat without damaging barley. The synthesis of I is given.

IT 52756-24-8F

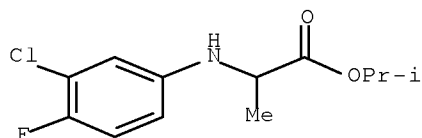
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and benzoylation of)

RN 52756-24-8 ZCAPLUS

CN Alanine, N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester (CA INDEX

10/598508

(NAME)



L58 ANSWER 95 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1975:579612 ZCAPLUS Full-text
 DOCUMENT NUMBER: 83:179612
 ORIGINAL REFERENCE NO.: 83:28225a,28228a
 TITLE: Herbicidal N,N-disubstituted alanine derivatives
 INVENTOR(S): Haddock, Ernest; Rossinger, Herbert P.
 PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.,
 Neth.
 SOURCE: Ger. Offen., 15 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2460691	A1	19750710	DE 1974-2460691	19741220
DE 2460691	C2	19830601		
CA 1049034	A1	19790220	CA 1974-214550	19741125
JP 50096537	A	19750731	JP 1974-146688	19741220
FR 2256913	A1	19750801	FR 1974-42267	19741220
DD 116743	A5	19751212	DD 1974-183275	19741220
AU 7476717	A	19760624	AU 1974-76717	19741220
ES 433186	A1	19770216	ES 1974-433186	19741220
GB 1488040	A	19771005	GB 1974-677	19741220
CH 611125	A5	19790531	CH 1974-17129	19741220
BE 823751	A2	19750623	BE 1974-1006352	19741223
NL 7416762	A	19750709	NL 1974-16762	19741223
NL 180582	B	19861016		
NL 180582	C	19870316		
US 3994713	A	19761130	US 1975-539201	19750106

PRIORITY APPLN. INFO.: GB 1974-677 A 19740107

AB 3,4-F2C6H3NBzCHMeCO2R (I; R = Me, Et, Me2CH) were prepared by heating BzCl with 3,4-F2C6H3NHCHMeCO2R in PhMe. I were useful as herbicides; test data were given.

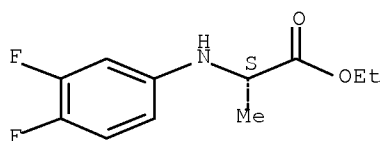
IT 57081-14-8 57081-16-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with benzoyl chloride)

RN 57081-14-8 ZCAPLUS

CN L-Alanine, N-(3,4-difluorophenyl)-, ethyl ester (CA INDEX NAME)

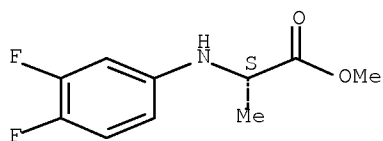
Absolute stereochemistry.

10/598508



RN 57081-16-0 ZCAPLUS
CN L-Alanine, N-(3,4-difluorophenyl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 96 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1975:543023 ZCAPLUS Full-text
DOCUMENT NUMBER: 83:143023
ORIGINAL REFERENCE NO.: 83:22461a,22464a
TITLE: Cyanomethylanilide herbicides
INVENTOR(S): Ito, Shigekazu; Wakamori, Shigeki; Kimura, Ichiro;
Takita, Kiyoshi
PATENT ASSIGNEE(S): Kumiai Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50077532	A	19750624	JP 1973-128668	19731115

PRIORITY APPLN. INFO.: JP 1973-128668 A 19731115

GI For diagram(s), see printed CA Issue.

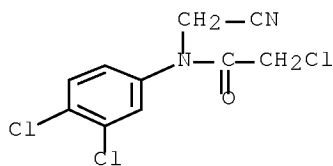
AB N-Cyanomethylanilides I (R = lower alkyl or Cl-substituted alkyl; X = H or Cl; n = 0-2) control weeds. Thus, when N-cyanomethyl- α -chloroacetanilide (I; R = ClCH₂; X = H; n = 1) [16272-49-4] was applied postemergence at 500 g/10 are to rice and to Echinochloa crus-galli, Monochoria vaginalis, Rotala indica, Dopetorium junceum, Eleocharis acicularis, Sagittaria pygmaea, and Scirpus juncoides in pot exts., all weeds were killed in 14 days, with no toxicity to rice. Synthesis of I is outlined.

IT 54590-53-3P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and herbicidal activity of)

RN 54590-53-3 ZCAPLUS

CN Acetamide, 2-chloro-N-(cyanomethyl)-N-(3,4-dichlorophenyl)- (CA INDEX NAME)



L58 ANSWER 97 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:517130 ZCAPLUS Full-text
 DOCUMENT NUMBER: 83:117130
 ORIGINAL REFERENCE NO.: 83:18423a,18426a
 TITLE: Antifouling marine paints
 INVENTOR(S): Kurono, Hitoshi; Hashimoto, Kensuke
 PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 49092134	A	19740903	JP 1972-103555	19721018
PRIORITY APPLN. INFO.:			JP 1972-103555	A 19721018

AB The antifouling marine paints contain derivs. of N-cyanomethyl-N-chloroacetylaniline having Me, MeO, NO₂, CF₃, and (or) ≤3 Cl substituents on the ring. Thus, a composition of N-chloroacetyl-N-cyanomethyl- 3,4-dichloroaniline 7.5, bis(triphenyltin)oxide [1262-21-1] 2.5, silica sand 8, plaster of Paris 4, red iron oxide 8, MeOH 3.2, drier 0.8, and boiled oil 66 weight% was diluted and applied to a steel plate. The plate was contaminated on 3 and 8% of the surface area after 3 and 6 months of immersion in the sea, resp., compared with 8 and 15%, resp., for a similar test with a paint containing 28.5% Cu₂O and 2% HgO. Similarly used was N-chloroacetyl-N-cyanomethyl-4-methylaniline [54590-54-4].

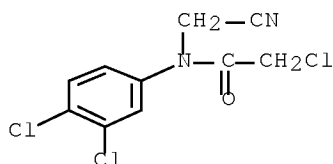
IT 54590-53-3

RL: USES (Uses)

(antifouling marine paints containing)

RN 54590-53-3 ZCAPLUS

CN Acetamide, 2-chloro-N-(cyanomethyl)-N-(3,4-dichlorophenyl)- (CA INDEX NAME)



L58 ANSWER 98 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:479158 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 83:79158

ORIGINAL REFERENCE NO.: 83:12427a,12430a

TITLE: Uses of sydnone for heterocyclic syntheses

AUTHOR(S): Badami, B. V.; Puranik, G. S.

CORPORATE SOURCE: Dep. Chem., Karnatak Univ., Dharwar, India

SOURCE: Canadian Journal of Chemistry (1975), 53(6), 913-14

CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 83:79158

GI For diagram(s), see printed CA Issue.

AB N-(4-Bromo-3-chlorophenyl)sydnone is prepared from 3,4-ClBrC₆H₃NHCH₂CO₂H and subjected to chlorination and bromination. 1,3-Dipolar addition of these sydnone with MeO₂CC...CCO₂Me produces substituted pyrazoles, e.g. I.

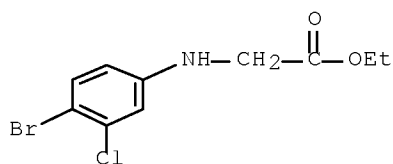
IT 56536-56-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 56536-56-2 ZCAPLUS

CN Glycine, N-(4-bromo-3-chlorophenyl)-, ethyl ester (CA INDEX NAME)



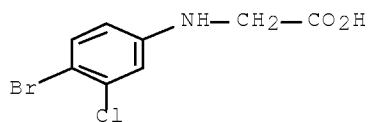
IT 56536-57-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and nitrosation of)

RN 56536-57-3 ZCAPLUS

CN Glycine, N-(4-bromo-3-chlorophenyl)- (CA INDEX NAME)



L58 ANSWER 99 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:156306 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 82:156306

ORIGINAL REFERENCE NO.: 82:24953a,24956a

TITLE: Ureidoimidazole fungicides

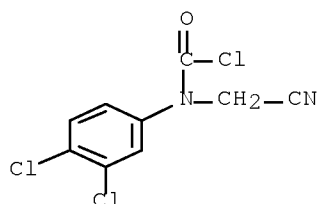
INVENTOR(S): Brookes, Robert F.; Godson, David H.; Hams, Anthony F.; Weighton, David M.; Wells, Wilfred Hase

10/598508

PATENT ASSIGNEE(S): Boots Co. Ltd.
 SOURCE: Ger. Offen., 65 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2429523	A1	19750116	DE 1974-2429523	19740620
DE 2429523	C2	19880721		
GB 1469772	A	19770406	GB 1973-29535	19730621
JP 50031047	A	19750327	JP 1974-70743	19740620
JP 60010003	B	19850314		
DD 113164	A5	19750520	DD 1974-179314	19740620
CS 188185	B2	19790228	CS 1974-4365	19740620
FR 2234293	A1	19750117	FR 1974-21739	19740621
US 3991071	A	19761109	US 1974-532667	19741213
ZA 7408037	A	19760128	ZA 1974-8037	19741218
US 4154945	A	19790515	US 1978-879564	19780221
PRIORITY APPLN. INFO.:			GB 1973-29535	A 19730621
			US 1974-477734	A2 19740610
			US 1974-6532667	A3 19741213
			US 1975-720880	A3 19760907

GI For diagram(s), see printed CA Issue.
 AB Approx. 250 title compds. (I, X = O, S, R1, R2 = e.g., Me, Et, allyl, Ph, CH2Ph, CH2CH2OPh) were prepared by refluxing imidazole with R1R2NCXCl, which was obtained from R1R2NH and COCl2 or CSCl2. Thus, PrBr was refluxed with AcNHC6H4Cl-2 in THF containing NaH to give 2-ClC6H4NHPr which was refluxed with COCl2 in EtOAc for 1.5 hr to give 2-ClC6H4NPrCOCl (II). Imidazole and II were refluxed 5 hr in THF containing Et3N to give I (X = O, R1 = Pr, R2 = C6H4Cl-2. Effective fungicidal quantities of I were given.
 IT 55240-14-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction with imidazole)
 RN 55240-14-7 ZCAPLUS
 CN Carbamic chloride, (cyanomethyl)(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)



L58 ANSWER 100 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1975:43316 ZCAPLUS Full-text
 DOCUMENT NUMBER: 82:43316
 ORIGINAL REFERENCE NO.: 82:6897a,6900a
 TITLE: Synthesis of antifols related to 2,4-diamino-6,7-

dihydro-5H-pyrrolo-[3,4-d]pyrimidine. Enhancement of antiparasitic selectivity by nitrogen linked mono and dichlorobenzoyl groups or the 3,4-dichlorophenylthiocarbamoyl group

AUTHOR(S): Southwick, Philip L.; Amarnath, Venkataraman; Madhav, R.

CORPORATE SOURCE: Dep. Chem., Carnegie-Mellon Univ., Pittsburgh, PA, USA

SOURCE: Journal of Heterocyclic Chemistry (1974), 11(5), 723-30
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

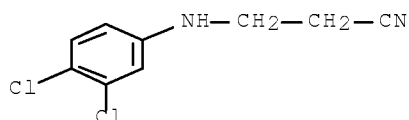
OTHER SOURCE(S): CASREACT 82:43316

AB 2,4-Diamino-6,7-dihydro-5H-pyrrolo[3,4-d]pyrimidine (I), its 7-Me (II), and 6-(chloro-substituted phenyl) derivs. were prepared Direct acylation of I and II with acid chlorides or mixed anhydrides gave 6-(chloro-substituted benzoyl or cinnamoyl) derivs. LiAlH₄ reduction of 6-(chloro-substituted benzoyl) derivs. under controlled conditions gave 6-(chloro-substituted benzyl) derivs. I also reacted with aryl isothiocyanates to yield 6-arylthiocarbamoyl derivs. Antimalarial assays, in vivo, against Plasmodium berghei and Plasmodium gallinaceum revealed that a somewhat enhanced in vivo antiparasitic effect above that of I without any evident increase in host toxicity was conferred by introduction of certain of the 6-chloro-substituted benzoyl groups or the 6-(3,4-dichlorophenyl-thiocarbamoyl) group. Corresponding 6-(chloro-substituted benzyl) derivs. more frequently displayed host toxicity.

IT 36053-75-5F
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with bromoacetate)

RN 36053-75-5 ZCAPLUS

CN Propanenitrile, 3-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 101 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:425391 ZCAPLUS Full-text

DOCUMENT NUMBER: 81:25391

ORIGINAL REFERENCE NO.: 81:4093a, 4096a

TITLE: Herbicidal alkyl 2-[benzoyl(3-chloro-4-fluorophenyl)amino]propionates

INVENTOR(S): Haddock, Ernest; Sampson, Alan J.

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.

SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2349970	A1	19740418	DE 1973-2349970	19731004

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DE 2349970	C2	19820916		
CA 1006003	A1	19770301	CA 1973-180776	19730911
BE 805652	A1	19740404	BE 1973-136333	19731004
NL 7313634	A	19740409	NL 1973-13634	19731004
FR 2202079	A1	19740503	FR 1973-35490	19731004
ZA 7307784	A	19740828	ZA 1973-7784	19731004
DD 108444	A5	19740920	DD 1973-173869	19731004
JP 49132232	A	19741218	JP 1973-111047	19731004
JP 56024641	B	19810608		
IT 998709	B	19760220	IT 1973-29737	19731004
CS 166653	B2	19760329	CS 1973-6840	19731004
GB 1437711	A	19760603	GB 1973-6464	19731004
ES 419329	A1	19760716	ES 1973-419329	19731004
CH 583507	A5	19770114	CH 1973-14188	19731004
DK 135712	B	19770613	DK 1973-5404	19731004
NO 138882	C	19781129	NO 1973-3866	19731004
NO 138882	B	19780821		
SU 664527	A3	19790525	SU 1973-1962504	19731004
SE 409704	B	19790903	SE 1973-13560	19731004
PRIORITY APPLN. INFO.:			GB 1972-46223	A 19721006
			GB 1973-6464	A 19730209

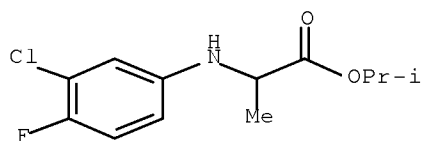
AB 3,4-ClFC6H3NBzCHMeCO2R (R = Me or CHMe2), used for the control of Avena fatua in cereal cultures, especially wheat and barley, were prepared by benzoylation of 3,4-Cl-FC6H3NHCHMeCO2R (I) with BzCl in PhMe at reflux. I were prepared from 3,4-ClFC6H3NH2 and ClCHMe2CO2H via 3,4-ClFC6- H3NHCHMeCO2H, followed by esterification.

IT 52756-24-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 52756-24-8 ZCAPLUS

CN Alanine, N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester (CA INDEX NAME)



L58 ANSWER 102 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:108210 ZCAPLUS Full-text

DOCUMENT NUMBER: 80:108210

ORIGINAL REFERENCE NO.: 80:17395a,17398a

TITLE: Herbicidal ethyl N-benzoyl-3,4-dichloroanilinopropionimide monhydrochloride

INVENTOR(S): Montijn, Paulus P.; Haddock, Ernest

PATENT ASSIGNEE(S): Shell Oil Co.

SOURCE: U.S., 2 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

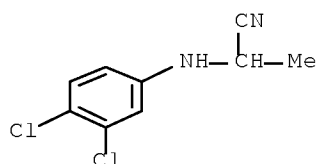
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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10/598508

 US 3790614 A 19740205 US 1971-205319 19711206
 PRIORITY APPLN. INFO.: GB 1971-59718 A 19710914
 GI For diagram(s), see printed CA Issue.
 AB The title ester (I) was prepared by the reaction of MeCH(NHC6H3Cl2-3,4)CN with BzCl followed by esterification of the resulting MeCH[N(C6H3Cl2- 3,4)Bz]CN with EtOH. At 0.05-5 kg/ha I was an effective herbicide against, e.g., wild oat.
 IT 28354-35-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with benzoyl chloride)
 RN 28354-35-0 ZCAPLUS
 CN Propanenitrile, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 103 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1974:59719 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 80:59719
 ORIGINAL REFERENCE NO.: 80:9681a,9684a
 TITLE: Herbicidal N-substituted N-phenylamines
 INVENTOR(S): Clayton, Anthony B.; Lehman, Stanley K.
 PATENT ASSIGNEE(S): Hercules Inc.
 SOURCE: Ger. Offen., 49 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2311897	A1	19731004	DE 1973-2311897	19730309
CA 1013960	A1	19770719	CA 1973-160333	19730102
CA 1257608	A1	19890718	CA 1973-160332	19730102
ZA 7300316	A	19731031	ZA 1973-316	19730116
AU 7351831	A	19740808	AU 1973-51831	19730205
DK 140082	C	19791119	DK 1973-725	19730209
DK 140082	B	19791119		
ES 411527	A3	19760101	ES 1973-411527	19730212
JP 49000232	A	19740105	JP 1973-20314	19730221
BE 796263	A1	19730702	BE 1973-128358	19730305
GB 1417273	A	19751210	GB 1973-10971	19730307
FR 2176075	A1	19731026	FR 1973-9209	19730308
FR 2176075	B1	19790511		
NL 7303363	A	19730912	NL 1973-3363	19730309
NL 178248	B	19850916		
NL 178248	C	19860217		
IT 981287	B	19741010	IT 1973-21429	19730309

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IT 981288	B	19741010	IT 1973-21430	19730309
CH 578830	A5	19760831	CH 1973-3525	19730309
AT 7302088	A	19770215	AT 1973-2088	19730309
AT 339284	B	19771010		
HU 170006	B	19770328	HU 1973-HE628	19730309
CH 602594	A5	19780731	CH 1975-7022	19730309
SU 1001847	A3	19830228	SU 1973-1894761	19730309
JP 48099341	A	19731215	JP 1973-28471	19730310
PL 94343	B1	19770730	PL 1973-161187	19730310
PL 100047	B1	19780831	PL 1973-191942	19730310
PL 101581	B1	19790131	PL 1973-201129	19730310
PL 101587	B1	19790131	PL 1973-201130	19730310
RO 68549	A1	19810924	RO 1973-74131	19730310
RO 69047	A1	19820510	RO 1973-86866	19730310
SE 411206	B	19750212	SE 1975-1572	19750212
SE 411206	C	19800327		
SE 7510667	A	19750923	SE 1975-10667	19750923
AT 349827	B	19790212	AT 1975-8102	19751023
AT 7803708	A	19800115	AT 1978-3708	19780522
AT 358322	B	19800910		
AT 7803707	A	19800915	AT 1978-3707	19780522
AT 362185	B	19810427		
AT 8003146	A	19801115	AT 1980-3146	19800613
AT 362958	B	19810625		
AT 8003147	A	19801115	AT 1980-3147	19800613
AT 362959	B	19810625		

PRIORITY APPLN. INFO.:

US 1972-233817	A	19720310
US 1972-233818	A	19720310
AT 1973-2088	A	19730309
CH 1973-3525	A	19730309

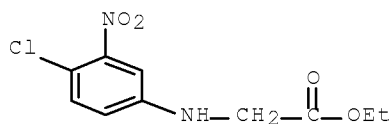
AB RNHCH2CO2Et [I; R = e.g., 4-ClC6H4, 2,4-Cl(O2N)C6H3, 2,4,5-Cl3C6H2, 3,2-Cl(MeO)C6H3] were prepared by the reaction of BrCH2CO2Et with RNH2. I reacted with R1CH2COCl (R1 = ClCH2, Cl2CH, Cl3C) to give R1CH2CONRCH2CO2Et (II). About 60 I and II were prepared, which were useful as herbicides.

IT 51114-23-9 51114-28-4 51114-31-9
51114-36-4 51114-38-6 51114-41-1
51114-44-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(herbicidal activity of)

RN 51114-23-9 ZCAPLUS

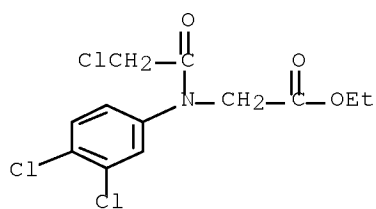
CN Glycine, N-(4-chloro-3-nitrophenyl)-, ethyl ester (CA INDEX NAME)



RN 51114-28-4 ZCAPLUS

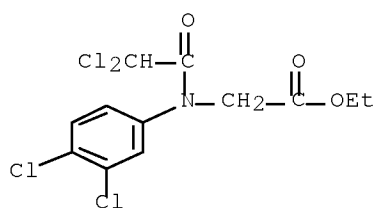
CN Glycine, N-(chloroacetyl)-N-(3,4-dichlorophenyl)-, ethyl ester (9CI) (CA INDEX NAME)

10/598508



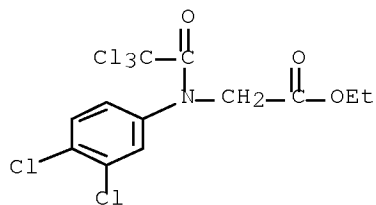
RN 51114-31-9 ZCAPLUS

CN Glycine, N-(dichloroacetyl)-N-(3,4-dichlorophenyl)-, ethyl ester (9CI)
(CA INDEX NAME)



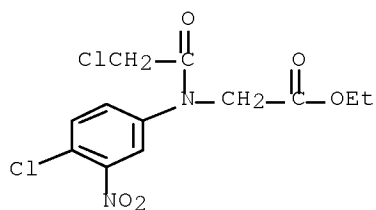
RN 51114-36-4 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)-N-(trichloroacetyl)-, ethyl ester (9CI)
(CA INDEX NAME)



RN 51114-38-6 ZCAPLUS

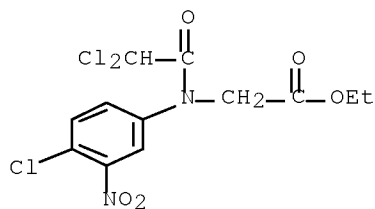
CN Glycine, N-(chloroacetyl)-N-(4-chloro-3-nitrophenyl)-, ethyl ester (9CI)
(CA INDEX NAME)



10/598508

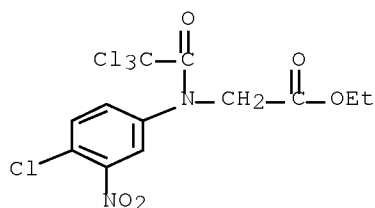
RN 51114-41-1 ZCAPLUS

CN Glycine, N-(4-chloro-3-nitrophenyl)-N-(dichloroacetyl)-, ethyl ester (9CI)
(CA INDEX NAME)



RN 51114-44-4 ZCAPLUS

CN Glycine, N-(4-chloro-3-nitrophenyl)-N-(trichloroacetyl)-, ethyl ester
(9CI) (CA INDEX NAME)



L58 ANSWER 104 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:466044 ZCAPLUS Full-text

DOCUMENT NUMBER: 79:66044

ORIGINAL REFERENCE NO.: 79:10667a,10670a

TITLE: Herbicidal alkyl 2-(N-benzoylhaloanilino)(thio)propion
imidates

INVENTOR(S): Montijin, Paulus P.; Haddock, Ernest

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij N. V.

SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2162073	A1	19730620	DE 1971-2162073	19711214
DE 2162073	B2	19800529		
DE 2162073	C3	19810129		

PRIORITY APPLN. INFO.: DE 1971-2162073 A 19711214

AB Seven RnC6H5-nNBzCHMeC(:NH)XR1.HCl (Rn = 3,4-Cl2, 4-Cl, 3,4-FC1, 4-F; X = O, S; R1 = Et, Me, CHMe2) were prepared (58-95%) by reaction of RnC6H5-nNBzCHMeCN, obtained by benzoylation of the anilinopropionitriles, with R1XH

10/598508

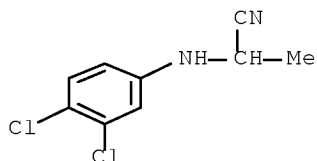
in EtOH-PhMe-Et₂O in the presence of HCl(g) at -20° and used as selective herbicides.

IT 28354-35-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(benzoylation of)

RN 28354-35-0 ZCAPLUS

CN Propanenitrile, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 105 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:438549 ZCAPLUS Full-text

DOCUMENT NUMBER: 79:38549

ORIGINAL REFERENCE NO.: 79:6235a,6238a

TITLE: Inhibition of histidine decarboxylase,
aromatic-L-amino acid decarboxylase, and acid
secretion by brocresine and its metabolites

AUTHOR(S): Ellenbogen, Leon; Kelly, Robert G.; Taylor, Russell
J., Jr.; Stubbs, Charles S., Jr.

CORPORATE SOURCE: Lederle Lab. Div., Am. Cyanamid Co., Pearl River, NY,
USA

SOURCE: Biochemical Pharmacology (1973), 22(8), 939-47
CODEN: BCPA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Brocresine (I) [555-65-7] and its metabolites, 4-bromo-3-hydroxybenzyl alc. [2737-19-1], 4-bromo-3-hydroxybenzoic acid [14348-38-0], and 4-bromo-3-hydroxyhippuric acid (II) [40771-10-6], inhibited rat fetal and rat gastric histidine decarboxylase [9024-61-7] in vitro with a molar I50 of approx. 10⁻⁸, 10⁻⁴, 10⁻³, and 10⁻⁵, resp., for enzymes; and inhibited aromatic-L-amino acid decarboxylase [9042-64-2] from hog kidney and rat gastric mucosa in vitro with a molar I50 of .sim.10⁻⁷, 10⁻⁴, 10⁻³, and 10⁻³, resp., for both enzymes. I, the alc. metabolite, and the acid metabolite inhibited rat gastric histidine decarboxylase after i.p. administration of 200 mg of compound per kg, whereas the hippurate was only weakly inhibitory. All 4 compds. inhibited gastric acid secretion in the pylorus-ligated rat, but the acid and hippurate were only moderately inhibitory. The reaction of hemoglobin with I to form methemoglobin explains the rapid disappearance of its inhibitory activity.

L58 ANSWER 106 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:132693 ZCAPLUS Full-text

DOCUMENT NUMBER: 78:132693

ORIGINAL REFERENCE NO.: 78:21295a,21298a

TITLE: Weed-controlling N,N-disubstituted amino acid
herbicides

INVENTOR(S): Yates, John; Payne, David H.

PATENT ASSIGNEE(S): Shell Oil Co.

SOURCE: U.S., 6 pp. Division of U.S. 3,598,859 (CA

10/598508

75;130132d).
CODEN: USXXAMDOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

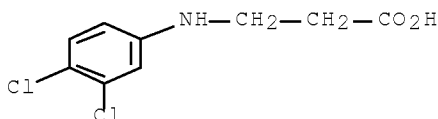
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3712805	A	19730123	US 1970-66094	19700821
US 3598859	A	19710810	US 1967-694116	19671228
PRIORITY APPLN. INFO.:			US 1967-694116	A3 19671228
			GB 1966-58406	A 19661230

AB Herbicide compns. containing N,N-disubstituted amino acids were tested for their ability to control wild oats and other weeds in cultivated areas. As an example, N-benzoyl-N-(3,4-dichlorophenyl)alanine ethyl ester (I) [33878-50-1], at 10 kg/ha, was highly phytotoxic to linseed mustard, and oats, but only slightly phytotoxic to corn, rye grass, and peas.

IT 31399-32-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloropropionic acid)

RN 31399-32-3 ZCAPLUS

CN β -Alanine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)

L58 ANSWER 107 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:110968 ZCAPLUS Full-text

DOCUMENT NUMBER: 78:110968

ORIGINAL REFERENCE NO.: 78:17807a,17810a

TITLE: Herbicidal alkyl 2-[N-(benzoyl)haloanilino]propionimides and -thiopropionimides

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij N. V.

SOURCE: Fr., 18 pp.
CODEN: FRXXAK

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2118588	A1	19720901	FR 1971-44848	19711214
JP 55029962	B	19800807	JP 1971-100784	19711214
SU 862811	A3	19810907	SU 1971-1726247	19711214
PRIORITY APPLN. INFO.:			GB 1970-59718	A 19701216

GI For diagram(s), see printed CA Issue.

AB The α -anilinopropionitriles (I, II, III, and IV) react with MeOH, EtOH, and Cl-3 alkyl mercaptans to give seven title esters (V; Q = O, S; R2 = Cl-3 alkyl), which are useful as herbicides.

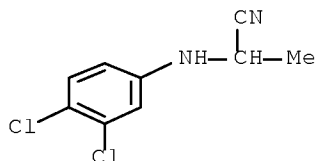
IT 28354-35-0

10/598508

RL: RCT (Reactant); RACT (Reactant or reagent)
(N-benzoylation of)

RN 28354-35-0 ZCAPLUS

CN Propanenitrile, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 108 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:43081 ZCAPLUS Full-text

DOCUMENT NUMBER: 78:43081

ORIGINAL REFERENCE NO.: 78:6803a,6806a

TITLE: α -(4-Haloanilino)propionic acid derivatives

INVENTOR(S): Montijn, Paulus Pieter; Van Helden, Robert; Haddock, Ernest

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij N. V.

SOURCE: Ger. Offen., 31 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

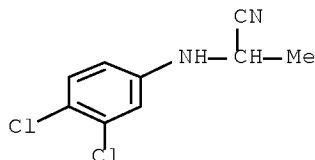
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

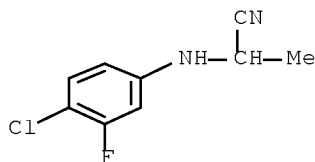
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2221109	A	19721116	DE 1972-2221109	19720428
DE 2221109	C2	19831006		
GB 1327294	A	19730822	GB 1971-12410	19710430
BE 782595	A2	19721025	BE 1972-3972	19720425
NL 7205688	A	19721101	NL 1972-5688	19720427
NL 175173	B	19840501		
NL 175173	C	19841001		
DK 153472	B	19880718	DK 1972-2127	19720427
DK 153472	C	19881121		
FR 2139847	A1	19730112	FR 1972-15325	19720428
IT 953845	B	19730810	IT 1972-23696	19720428
AU 7241680	A	19731101	AU 1972-41680	19720428
DD 101889	A5	19731120	DD 1972-162648	19720428
HU 164835	B	19740411	HU 1972-SE1623	19720428
SU 461492	A3	19750225	SU 1972-1778332	19720428
PL 83652	B1	19751231	PL 1972-155049	19720428
ES 402224	A1	19760101	ES 1972-402224	19720428
CA 982141	A1	19760120	CA 1972-140875	19720428
CH 589049	A5	19770630	CH 1972-6395	19720428
RO 62750	A1	19771015	RO 1972-70736	19720428
CS 195255	B2	19800131	CS 1972-2895	19720428
JP 57049537	B	19821022	JP 1972-42319	19720428
JP 56039057	A	19810414	JP 1980-103781	19800730
JP 57036274	B	19820803		
PRIORITY APPLN. INFO.:			GB 1971-12410	A 19710430

10/598508

GI For diagram(s), see printed CA Issue.
AB Six title propionic acid derivs. (I; R = H, Bz; R1 = CN, CO2Et; R2 = Cl, F; R3 = H, Cl, F), useful herbicides, were prepared in 73-91.7% yields by reaction of 4,3-R2R3C6H3NH2 with AcH and HCN or with HOCHMeCN, optionally followed by reaction with EtOH-HCl and BzCl.
IT 28354-35-0P 39234-77-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28354-35-0 ZCAPLUS
CN Propanenitrile, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



RN 39234-77-0 ZCAPLUS
CN Propanenitrile, 2-[(4-chloro-3-fluorophenyl)amino]- (CA INDEX NAME)

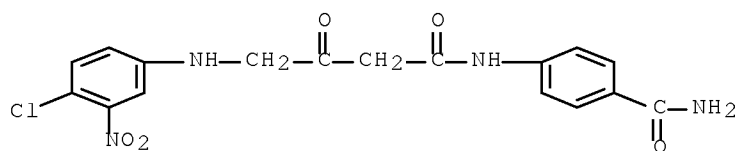


L58 ANSWER 109 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:548142 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 77:148142
ORIGINAL REFERENCE NO.: 77:24327a,24330a
TITLE: Toxicity of acetoacetic acid nitrocarbamoylanilide derivatives based on experimental tests
AUTHOR(S): Evstatieva, M. M.
CORPORATE SOURCE: USSR
SOURCE: Gig. Primen., Toksikol. Pestits. Klin. Otravl. (1971), No. 9, 356-60
From: Ref. Zh., Biol. Khim. 1972, Abstr. No. 6F2167
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Acetoacetic acid m-nitro-p-aniline-4-carbamoylanilide [36894-78-7], acetoacetic acid o-nitroaniline-4-carbamoylanilide [36894-79-8], and acetoacetic acid p-chloro-o-nitroaniline-4-carbamoylanilide [36894-80-1] (in 96 doses of 500 mg/kg, during 120 days) caused changes in mice respiratory enzymes, indicative of their toxicity, and induced temporary changes in hemoglobin concns. I also caused leukopenia.
IT 36894-78-7
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of)

10/598508

RN 36894-78-7 ZCAPLUS

CN Benzamide, 4-[[4-[(4-chloro-3-nitrophenyl)amino]-1,3-dioxobutyl]amino]-
(CA INDEX NAME)



L58 ANSWER 110 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1972:140459 ZCAPLUS Full-text

DOCUMENT NUMBER: 76:140459

ORIGINAL REFERENCE NO.: 76:22791a

TITLE: Reactions of nitriles. VIII. Synthesis of
2,3-dihydro-4(1H)-quinolinones

AUTHOR(S): Merchant, J. R.; Chothia, D. S.

CORPORATE SOURCE: Inst. Sci., Bombay, India

SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1972-1999)
(1972), (7), 932-5

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 76:140459

GI For diagram(s), see printed CA Issue.

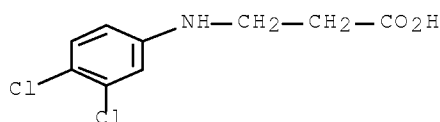
AB Cyanoethylation of 18 alkyl- and alkoxyanilines with CH₂:CHCN in AcOH gave the
corresponding β-anilinopropiononitriles, which were hydrolyzed to the
corresponding acids and cyclized to 2,3-dihydro-4(1H)-quinolinones; e.g., o-
MeOC₆H₄NH(CH₂)₂CO₂H cyclized to give 87% 2,3-dihydro-8-methoxy- 4(1H)-
quinolinone (I).

IT 31399-32-3P 36053-75-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

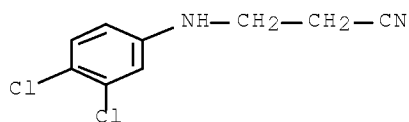
RN 31399-32-3 ZCAPLUS

CN β-Alanine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)



RN 36053-75-5 ZCAPLUS

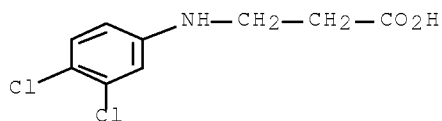
CN Propanenitrile, 3-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 111 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1972:45895 ZCAPLUS Full-text
 DOCUMENT NUMBER: 76:45895
 ORIGINAL REFERENCE NO.: 76:7401a,7404a
 TITLE: Reactions of acrylic acid with aromatic amines
 AUTHOR(S): Golovyashkina, L. F.; Grivtsova, L. N.
 CORPORATE SOURCE: Inst. Khim. Rast. Veshch., Tashkent, USSR
 SOURCE: Uzbekskii Khimicheskii Zhurnal (1971), 15(5), 79-81
 CODEN: UZKZAC
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian

AB From the reaction of 1 mole $\text{CH}_2\text{:CHCO}_2\text{H}$ (I) with 1 mole $\text{XC}_6\text{H}_4\text{NH}_2$ (II) at $85-90^\circ$ ($40-5^\circ$ in the case $\text{X}=\text{p-Me}$), $\text{XC}_6\text{H}_4\text{NH}(\text{CH}_2)_2\text{CO}_2\text{H}$ (III, $\text{X}=\text{p-Me}$, p-NO_2 , $3,4\text{-Cl}_2$, Ph) were obtained in 70, 98, 72, and 33% yields. At 1:2 (molar) I-II and $180-90^\circ$ ($85-90^\circ$ in the case $\text{X}=\text{p-Me}$), the products ($\text{XC}_6\text{H}_4\text{NH}(\text{CH}_2)_2\text{CONHC}_6\text{H}_4\text{X}$, $\text{X}=\text{p-Me}$, p-NO_2 , $3,4\text{-Cl}_2$), prepared in 64, 37, and 60% yield, were identical with those obtained from the reaction of $\text{CH}_2\text{:CHCONHC}_6\text{H}_4\text{X}$ with II and were not obtained when III reacted under the same conditions with II, except in the case $\text{X}=\text{p-NO}_2$ and then only in 5% yield.

IT 31399-32-3F
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 31399-32-3 ZCAPLUS
 CN β -Alanine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)



L58 ANSWER 112 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1971:551656 ZCAPLUS Full-text
 DOCUMENT NUMBER: 75:151656
 ORIGINAL REFERENCE NO.: 75:23917a,23920a
 TITLE: Azabenzocycloheptenones. XIII. Ring expansion of 1,2-dihydroquinoline derivatives
 AUTHOR(S): Cromarty, A.; Haque, K. E.; Proctor, G. R.
 CORPORATE SOURCE: Dep. Pure Appl. Chem., Univ. Strathclyde, Glasgow, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (21), 3536-40
 CODEN: JSOOAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 75:151656

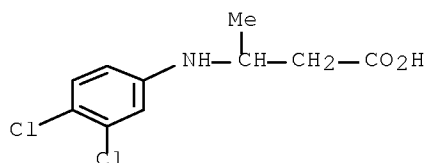
10/598508

AB Dibromocarbene reacted with 4-ethoxy-1,2-dihydro-1-(p-tolylsulfonyl)quinolines to give adducts which were converted into 4-bromo-5-ethoxy-1-(p-tolylsulfonyl)-1-benzazepines and into 4-bromo-1,2-dihydro-1-(p-tolylsulfonyl)-1-benzazepin-5-ones. 4-Ethoxy-1,2-dihydro-2-methyl-1-(p-tolylsulfonyl)-quinolines did not react with dihalocarbenes, but 4-ethoxy-1,2-dihydro-2-methyl-1-(methylsulfonyl)quinoline reacted with dibromocarbene to give an adduct which was ring-expanded to 2-methyl-1-benzazepine derivs.

IT 34129-52-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 34129-52-7 ZCAPLUS

CN Butanoic acid, 3-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 113 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:99994 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 74:99994

ORIGINAL REFERENCE NO.: 74:16281a,16284a

TITLE: 2-Amino-4-hydroxy-6-arylaminioethylpteridines as potential antimalarial agents

AUTHOR(S): DeGraw, Joseph I.; Brown, Vernon H.; Cory, M.; Tsakotellis, Panayotis; Kisliuk, Roy L.; Gaumont, Yvette

CORPORATE SOURCE: Dep. Pharm. Chem., Stanford Res. Inst., Menlo Park, CA, USA

SOURCE: Journal of Medicinal Chemistry (1971), 14(3), 206-10
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

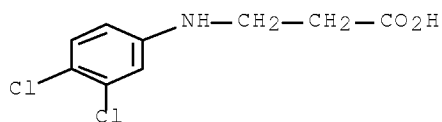
GI For diagram(s), see printed CA Issue.

AB 2-Amino-4-hydroxy-6-arylaminioethylpteridines (I), including homopteroic acid (I, R = p-CO₂H), were prepared by condensation of 2-amino-4-hydroxy-5-phenylazo-6-chloropyrimidine with amino semicarbazones [ArN(Ac)CH₂CH₂C(:NNHCONH₂)CH₂NH₂.-HX] to give 2-amino-4-hydroxy-5-phenylazo-6-pyrimidinylamino ketones (II). Catalytic reduction of the phenylazo moiety was accompanied by ring closure to the 7,8-dihydropteridine which could be aromatized by oxidation in situ with H₂O₂. I were inactive against Plasmodium berghei in rodents, possibly due to poor cell permeability. However, homopteroic acid significantly inhibited the growth of Streptococcus faecium by blocking the folic acid uptake.

IT 31399-32-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 31399-32-3 ZCAPLUS

CN β-Alanine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)



L58 ANSWER 114 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1970:132335 ZCAPLUS Full-text
 DOCUMENT NUMBER: 72:132335
 ORIGINAL REFERENCE NO.: 72:23683a,23686a
 TITLE: Anticonvulsant and muscle relaxant
 2-(p-substituted-phenyl)-2-methylbutyramides
 INVENTOR(S): Thorp, Jeffrey M.; Waring, Wilson S.
 PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
 SOURCE: Brit., 8 pp.
 CODEN: BRXXAA
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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GB 1177548		19700114	GB 1967-5412467	19671128

GI For diagram(s), see printed CA Issue.

AB A mixture of 10 g α -(p-chlorophenoxy)- α -methylbutyric acid and 10 ml SOCl₂ was refluxed 20 min and the product treated with NH₃ to give I (R = p-Cl, R₁ = Me, R₂ = NH₂) (II). Also prepared were I (R₁ = Me) (R, R₂, b.p., and m.p. given): p-Cl, HNMe, -, 75-6° (petroleum ether b. 40-60°); p-Cl, NMe₂, 103-6°/0.2 mm, 62-4° (petroleum ether); p-Br, NH₂, -, 73° (cyclohexane). A stirred solution of 17.3 g p-BrC₆H₄OH in 200 ml dry xylene was treated with 5 g (50% dispersion in oil) NaH at a rate to keep the temperature <20°, the temperature was raised to 130°, and the mixture treated dropwise with 22 g Et α -bromo- α -methylbutyrate at 160° and stirred 2 hr at 125-30° to give I (R = p-Br, R₁ = Me, R₂ = OEt), b.p. 100-5°; acid m. 96-7° (petroleum ether). Also prepared were I (R₁ = Me) (R, R₂, b.p., and m.p. given): p-Me, NH₂, -, 65-6° (petroleum ether); p-Me, OEt, 80-5°/0.15 mm, -; p-Me, OH, -, - (oil); p-OMe, NH₂, -, 73-5° (petroleum ether); p-OMe, OEt, 100-2°/0.2 mm, -; p-OMe, OH, -, - (oil). α -(p-Chloroanilino)- α -methylbutyronitrile (15 g) was added to 40 ml concentrated H₂SO₄ and the mixture stirred 18 hr at room temperature, and alkalinized with aqueous NH₄OH to give α -(p-chloroanilino)- α -methylbutyramide (III, R = H, R₁ = p-Cl, R₂ = Me, R₃ = CONH₂), m. 88-9° (EtOH). Also prepared were III (R, R₁, R₂, R₃, and m.p. given): H, p-Cl, Et, CONH₂, 111-12° (C₆H₆); 3-Cl, 4-Cl, Me, CONH₂, 115-16° (C₆H₆); H, 4-Bu, Me, CN, - (oil). A stirred mixture of 12.7 g p-ClC₆H₄NH₂, 7.2 g MeCOEt, and 40 ml HOAc was treated with 4.9 g NaCN and 25 ml H₂O and the mixture stirred 30 min to give III (R = H, R₁ = p-Cl, R₂ = Me, R₃ = CN), m. 103-4° (MeOH). Also prepared were α -(p-chloroanilino)- α -methylvaleramide, m. 107-8° (petroleum ether), and the nitrile, m. 83-4° (EtOH). A mixture of Et α -(p-chlorophenoxy)- α -methylbutyrate (IV) (2 g), 2 g hydrazine, and 4 ml EtOH was refluxed 36 hr and worked up to give α -(p-chlorophenoxy)- α -methylbutyrylhydrazide; HCl salt m. 169-70°. Na (0.9 g) was dissolved in 25 ml EtOH; half of the NaOEt solution was added to 2.8 g H₂NOH.HCl in 12 ml hot EtOH, the mixture cooled, filtered, the filtrate treated with 5 g IV and the remainder of the NaOEt and the mixture kept 9 days

10/598508

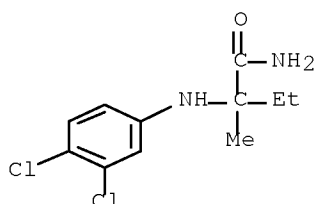
at room temperature to give I (R = p-Cl, R1 = Me, R2 = NHOH), m. 113-14° (C6H6). NaH (1.4 g, 50% suspension in oil) was added to 3.8 g p-ClC6H4OH in dry HCONMe2 (DMF) at 5°, the mixture stirred 30 min at room temperature, treated dropwise with 5.3 g α-bromo-α-methylbutyramide in 10 ml DMF, and the mixture stirred 12 hr at room temperature and heated 1 hr at 60-70° to give II, m. 68-9° (petroleum ether). A mixture of 4.1 g Me α-(p-chlorophenoxy)-α-methylbutyrate and MeOH-NH3 (25 ml saturated solution at 20°) was heated 72 hr in a sealed tube at 110° to give II, m. 68-9°. These compds. possess central nervous system depressant activity.

IT 28139-34-6P 28139-37-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

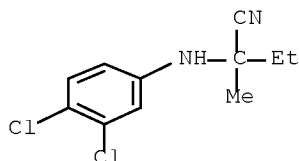
RN 28139-34-6 ZCAPLUS

CN Butyramide, 2-(3,4-dichloroanilino)-2-methyl- (8CI) (CA INDEX NAME)



RN 28139-37-9 ZCAPLUS

CN Butyronitrile, 2-(3,4-dichloroanilino)-2-methyl- (8CI) (CA INDEX NAME)



L58 ANSWER 115 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:21042 ZCAPLUS Full-text

DOCUMENT NUMBER: 72:21042

ORIGINAL REFERENCE NO.: 72:3825a,3828a

TITLE: Nitration inhibitors in soil

INVENTOR(S): Hojo, Shiro; Doya, Masaharu; Iesaka, Hiroyuki

PATENT ASSIGNEE(S): Japan Gas-Chemical Co., Inc.

SOURCE: Jpn. Tokkyo Koho, 9 pp.

CODEN: JAXXAD

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

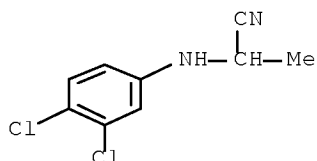
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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10/598508

JP 44013971 B4 19690621 JP 19661212
 AB RNHCHR1CN [I, R = substituted (halo, alkyl, alkoxy)-phenyl, naphthyl, or biphenyl, R1 = H or Me, 58 compds.] are used as the title materials. For example, a mixture of equal amts. of soil and nitration bacteria-saturated sand containing 20 mg (NH4)2CO3/100 g dry soil (or urea) and 100 ppm I (R = Ph, R1 = H) showed a nitration inhibition efficiency of 61% or 2.6 mg N (nitrate) after incubation at 28° for 48 hrs.
 IT 28354-35-0
 RL: BIOL (Biological study)
 (nitrate formation inhibitors)
 RN 28354-35-0 ZCAPLUS
 CN Propanenitrile, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 116 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1968:467079 ZCAPLUS Full-text
 DOCUMENT NUMBER: 69:67079
 ORIGINAL REFERENCE NO.: 69:12515a,12518a
 TITLE: Herbicidal anilinoalkanamides
 PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij N. V.
 SOURCE: Neth. Appl., 41 pp.
 CODEN: NAXXAN
 DOCUMENT TYPE: Patent
 LANGUAGE: Dutch
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6707890		19671211	NL 1967-7890	19670607
DE 1642337			DE	
FR 1525715			FR	
GB 1122043			GB	
US 3634509		19720111	US	19690903
US 3734711		19730522	US	19710315
PRIORITY APPLN. INFO.:			GB	19660608
			GB	19670502

GI For diagram(s), see printed CA Issue.
 AB The title compds. of the general formula I, where the symbols have the tabulated values, were prepared either by treating the corresponding chlorobenzene with the corresponding amino acid in EtOH in the presence of NaHCO3 at 70-120°, refluxing the formed acid in C6H6 with thionyl chloride (II), and treating the formed acid chloride with the corresponding amine in CH2Cl2 at a temperature between -20° and +30°, or by treating the corresponding aniline with the corresponding BrCHR(CH2)nCO2Et at 80-120°, and treating the formed ester with the corresponding amine in EtOH at 100-50°. Thus, a mixture of 1-chloro-2,6-dinitrobenzene 810, DL-alanine 384, and NaHCO3 840 g. was

stirred and refluxed 18 hrs. in 8 l. 95% EtOH and the mixture diluted with 4 l. water, filtered, distilled in vacuo while adding 4 l. water to remove EtOH, cooled by adding 2 l. ice, acidified with concentrated HCl, and stirred to give 95% 2-(2,6-dinitroanilino)propionic acid (III), m. 137-8°. To a solution of 490 g. III in 2.5 l. C₆H₆ 570 g. II was added while stirring and the mixture stirred and refluxed 12 hrs., filtered, and distilled to remove C₆H₆ and excess II. To a solution of the residual oil in 2.5 l. CH₂Cl₂, a solution of 160 g. NH₂Me in 1 l. CH₂Cl₂ was added while stirring at 0-5°, the mixture filtered, the filtrate evaporated, and the residue stirred with 1 l. tech. denaturated alc. to give 61% I (X₂ = X₆ = NO₂, X₃ = X₄ = X₅ = H, R = Me; n = 0, R₁ = H, R₂ = Me) m. 146-8°. Similarly prepared I are given in Table 1, page 6259. A mixture of 2,5-dichloroaniline 324 and ethyl 2-bromopropionate 18.1 g. was heated 5 hrs. at 100°, water added to the hot melt, the organic phase extracted with Et₂O, the extract evaporated, and the residue fractionally distilled in vacuo to give 7 g. ethyl 2-(2,5-dichloroanilino)propionate (IV), b_{0.9} 127-30°. IV (10 g.) was heated 15 hrs. at 120° with 50 cc. 33 weight/volume % solution of NH₂Me in EtOH in a closed tube and the reaction mixture was concentrated, filtered hot, and allowed to cool to give 70% I (X₂ = X₅ = Cl, X₃ = X₄ = X₆ = H, R = Me, n = 0, R₁ = H, R₂ = Me), m. 168-9° (EtOH). Similarly prepared I are given in Table 2.

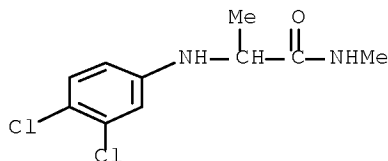
IT 19383-37-0 19386-55-1

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(as herbicide)

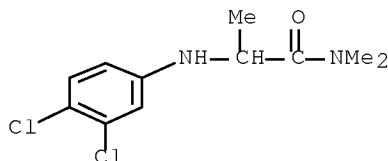
RN 19383-37-0 ZCAPLUS

CN Propionamide, 2-(3,4-dichloroanilino)-N-methyl- (8CI) (CA INDEX NAME)



RN 19386-55-1 ZCAPLUS

CN Propionamide, 2-(3,4-dichloroanilino)-N,N-dimethyl- (8CI) (CA INDEX NAME)



L58 ANSWER 117 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:499878 ZCAPLUS Full-text

DOCUMENT NUMBER: 67:99878

ORIGINAL REFERENCE NO.: 67:18767a,18770a

TITLE: Preparation of pesticides

10/598508

PATENT ASSIGNEE(S): Allied Chemical Corp.
 SOURCE: Neth. Appl., 31 pp.
 CODEN: NAXXAN
 DOCUMENT TYPE: Patent
 LANGUAGE: Dutch
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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NL 6608951		19670102	NL 1966-8951	19660628
DE 1543308			DE	
GB 1125299			GB	
GB 1125300			GB	
US 3420919		19690107	US	19650630
US 3499964		19700310	US	19680925
			US	19650630

PRIORITY APPLN. INFO.:

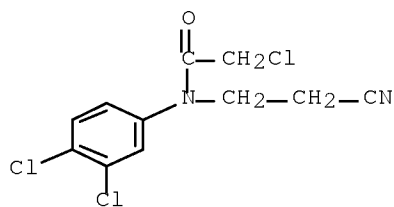
AB The cyano amide phosphate and phosphonate compds., (R1O)R2P(Y)SCH2CONZCnH2nCN (I), were prepared by reaction of a suitable alkylalkoxy- or dialkoxyphosphorodithioate, with a haloacetamidonitrile. Thus, 10 parts α -chloro-N-(cyanoethyl)-N-phenylacetamide is dissolved in 79.2 parts Me2CO, and a solution containing 11 parts NH4 O,O-diethylphosphorodithioate in 79.2 parts Me2CO is added, and the mixture stirred 45 hrs. yielding 16 parts α -(diethoxythionophosphinothio)-N-(2-cyanoethyl)-N-phenylacetamide, viscous oil. The haloacetamidonitrile was prepared as follows. To 36.5 parts 3-anilinopropionitrile and 8.0 parts Et2O was added 20 parts pyridine in 8.0 parts Et2O. After cooling to 20°, while stirring, 28.3 parts chloroacetyl chloride in 60 parts ethyl ether was added slowly, after which the mixture was stirred 18 hrs. at room temperature, 300 parts H2O added, the solid filtered off and washed with H2O to yield 43.5 parts α -chloro-N-(2-cyanoethyl)-N-phenylacetamide (II), m. 67-9° (Et2O). Other prepared compds. were: α -(diethoxyphosphinothio)-N-phenylacetamide; α -(dimethoxythionophosphinothio)-N-phenylacetamide; α -(diethoxythionophosphinothio)-N-(2-chlorophenyl)acetamide; α -chloro-N-(2-cyanoethyl)-N-(2-chlorophenyl)acetamide; α -(dimethoxythionophosphinothio)-N-(2-cyanoethyl)-N-(2-chlorophenyl)acetamide; (diethoxyphosphinothio)-N-(2-cyanoethyl)-N-(2-chlorophenyl)acetamide; α -(diethoxythionophosphinothio)-N-(2-cyanoethyl)-N-(4-fluorophenyl)acetamide; α -chloro-N-(2-cyanoethyl)-N-(4-fluorophenyl)acetamide; α -(dimethoxythionophosphinothio)-N-(2-cyanoethyl)-N-(4-fluorophenyl)acetamide; α -(diethoxythionophosphinothio)-N-(2-cyanoethyl)-N-(3,4-dichlorophenyl)acetamide; α -chloro-N-(2-cyanoethyl)-N-(3,4-dichlorophenyl)acetamide. To test the toxicity, 4.8 g. II was dissolved in 100 ml. Me2CO. Thus, 1 weight part toxic compound/79 weight parts H2O give 100% control of Tetranychus telarius; 1 weight part toxic compound/639 weight parts H2O give 100% control of Epilachna varivestis, and 1 weight part toxic compound/159 weight parts H2O give 100% control of Prodenia eridania.

IT 16231-86-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 16231-86-0 ZCAPLUS

CN Acetanilide, 2,3',4'-trichloro-N-(2-cyanoethyl)- (8CI) (CA INDEX NAME)



L58 ANSWER 118 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:482381 ZCAPLUS Full-text

DOCUMENT NUMBER: 67:82381

ORIGINAL REFERENCE NO.: 67:15563a,15566a

TITLE: Synthesis and transformation of some N-phenylglycine derivatives

AUTHOR(S): Eckstein, Zygmunt; Plenkiewicz, Jan; Sak, Marek

CORPORATE SOURCE: Politech, Warsaw, Pol.

SOURCE: Roczniki Chemii (1967), 41(3), 493-502

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal

LANGUAGE: Polish

GI For diagram(s), see printed CA Issue.

AB N-Arylglycine Et esters and their derivs., such as N- arylaminoacetohydroxamic acids, Et N,N'-diarylhydantoates, and 1,3-diarylhydantoin, were prepared to test their antifungal activity against *Fusarium culmorum*, *Alternaria tenuis*, and *Rhizoctonia solani*. Thus, 0.1 mole ArNH₂, 0.1 mole AcONa, and 0.1 mole ClCH₂CO₂Et in 20 ml. EtOH was refluxed 8 hrs. to give ArNHCH₂CO₂Et (I) (method A). I were prepared from 0.1 mole ArNHCH₂CO₂H (II) in 30 ml. anhydrous EtOH, treated during 4 hrs. with dry HCl, then kept 24 hrs. at room temperature (method B). The following I were reported. (Ar, m.p., % yield, and method of preparation given): 4-IC₆H₄, 85-7°, 50, A; 3,4-ClMeC₆H₃, 91-3°, 57, A; 3,4-Cl(MeO)C₆H₃, 110-12°, 46, A; 3,4-I(MeO)C₆H₃, 109-10°, 53, A; 2,5-Cl₂C₆H₃, 30-1°, 38, B; 3,4-Cl₂C₆H₃, 104-6°, 64, A; 2,3,4-Cl₃C₆H₂, 61-3°, 38, B; 2,4,5-Cl₃C₆H₂, 77-8°, 41.5, B; 3,4,5-Cl₃C₆H₂, 135-7°, 48, A; 2,5,4-Cl₂BrC₆H₂, 76-8°, 53.5, B. 2,5-Cl₂C₆H₃NHAc (120 g.) in 400 ml. AcOH with a small amount of Fe dust and 90 ml. HCl was treated dropwise at 60° with an aqueous solution of 22.5 g. NaClO₃ to give 105 g. 2,4,5-Cl₃C₆H₂NHAc (III), m. 180-2° (C₆H₆). When hydrolyzed in 250 ml. EtOH and 70 ml. 30% NaOH, III gave 80 g. 2,4,5-trichloroaniline (IV), m. 92-4°. IV (40 g.) in 60 ml. EtOH was diluted with 18 g. 30% formalin and 1.5 g. 30% aqueous KOH, heated to 80°, and treated while vigorously stirring, with 13.5 g. KCN in 23 ml. water. The resulting mixture was heated 4.5 hrs. and acidified to give 52% II (Ar = 2,4,5-Cl₃C₆H₂) (V), m. 184-5°. Similarly prepared were II (Ar = 4-IC₆H₄), m. 121-3°, and II (Ar = 2,3,4-Cl₃H₆H₂), m. 206-8°, in 48 and 56% yields, resp. Oxidative chlorination of 21.8 g. II (Ar = 2,5-Cl₂C₆H₃) (VI) at 20° with NaClO₃ carried out as described above afforded 7.5 g. V. Similarly 21.8 g. VI in 120 ml. AcOH heated to 80°, then cooled to 18°, diluted with 24 ml. 40% HBr containing a small amount of Fe dust, and treated at 20° with 3.8 g. NaClO₃ in 5 ml. H₂O gave 17 g. II (Ar = 2,4,5-Cl₂BrC₆H₂), m. 187-9°. I (0.05 mole) in 30 ml. C₆H₆ and 6 g. PhNCO refluxed 10 hrs. gave PhNHCONArCH₂CO₂Et (VII), which were recrystd. from CCl₄. The following VII were reported (Ar, m.p., and % yield given): Ph (VIII), 108.5-109, 94°; 3-MeC₆H₄, 92.5-3.5°, 90; 4-MeC₆H₄, 99-100°, 98; 3-ClC₆H₄, 125-7°, 85; 4-ClC₆H₄, 130-2°, 97; 4-BrC₆H₄, 126.5-27°, 88; 3,4-Cl₂C₆H₃, 149-50°, 98. Ir spectra of these VII are reported. VIII (36.6 g.) in 30 ml. EtOH refluxed 3 hrs. and diluted while hot with alc. until the

mixture became clear gave 84% IX (Ar = Ph, R = H, X = O) (X), m. 138-9°. X was also prepared in three other ways: (a) quant. by heating VIII 5 min. at 170° in dimethylformamide (DMF); (b) quant. when VIII was refluxed 5 hrs. with MeONa; (c) in 75.5% yield from 3.32 g. PhNHCH₂CONHOH and 25 ml. DMF treated with 2.4 g. PhNCO in 7 ml. DMF, and heated 10 hrs. at 70°. The following IX were reported (Ar, R, X, m.p., and % yield given): 3-MeC₆H₄, H, O, 150-1.5°, 89; 4-MeC₆H₄, H, O, 166-8°; 82; 3-ClC₆H₄, H, O, 173.5-75°, 98; 4-ClC₆H₄, H, O, 173-5°, 90; 4-BrC₆H₄, H, O, 173-4°, 90; 3,4-ClC₆H₄, H, O, 191.5-93°, 88; Ph, H, S, 211-12°, 82; Ph, 4-Cl, S, 218-20°, 65. Hydroxylamine (prepared from 5.3 g. hydroxylamine-HCl in 35 ml. MeOH when treated with MeONa, obtained from 2.4 g. metallic Na in 50 ml. MeOH) was treated with 0.03 mole I and left 48 hrs. at room temperature to give the following ArNHCH₂CONHOH [Ar, m.p.

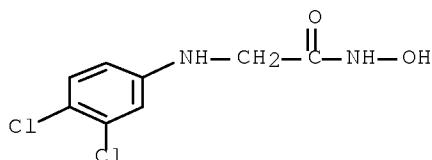
(decomposition), and % yield given]: Ph, 117-18°, 82; 4-FC₆H₄, 111.5-12°, 80; 2-ClC₆H₄, 122.5-23°, 80; 3-ClC₆H₄, 107.5-8.0°, 76; 4-ClC₆H₄, 97.5-98°, 75; 4-BrC₆H₄, 98-9°, 68; 3-IC₆H₄, 116-16.5°, 85; 4-IC₆H₄, 107.5-8.0°, 75; 4-O₂NC₆H₄, 132-3°, 51; 2-MeC₆H₄, 126.5-27°, 70; 3-MeC₆H₄, 109.5-10°, 63; 4-MeC₆H₄, 120.5-21°, 68; 2-EtC₆H₄, 104-5°, 79; 4-MeOC₆H₄, 136.5-7.5°, 74; 2,4-F₂C₆H₃, 118.5-19.5°, 65; 2,5-Cl₂C₆H₃, 136-7°, 85; 3,4-Cl₂C₆H₃, 110-11°, 83; 3,4-ClMeC₆H₃, 117-18°, 86; 3,4-Cl(MeO)C₆H₃, 135-6°, 88; 3,4-I(MeO)C₆H₃, 149-9.5°, 89; 2,3,4-Cl₃C₆H₂, 127.5-28°, 80; 2,4,5-Cl₃C₆H₂, 122.5-23°, 74; 3,4,5-Cl₃C₆H₂, 106-7.5°, 89; 2,5,4-Cl₂BrC₆H₂, 131.5-2.5°, 81.

IT 14108-53-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14108-53-3 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-hydroxy- (CA INDEX NAME)



L58 ANSWER 119 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:65821 ZCAPLUS Full-text

DOCUMENT NUMBER: 66:65821

ORIGINAL REFERENCE NO.: 66:12435a,12438a

TITLE: Properties and biological activity of some-N-aryl derivatives of aminoacetohydroxamic acid

AUTHOR(S): Eckstein, Zygmunt; Sak, Marek

CORPORATE SOURCE: Tech. Univ., Warsaw, Pol.

SOURCE: Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques (1966), 14(10), 745-50
CODEN: BAPCAQ; ISSN: 0001-4095

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Derivs. of ArNHCH₂CO₂Et (I) were prepared by the reactions (Takeda, CA 52, 5319h) of arylamines with either ClCH₂CO₂Et or HCHO and KCN followed by esterification of the intermediate N-aryl glycines. The treatment of N-(2,5-dichlorophenyl)glycine with NaClO₃/HCl and NaClO₃/HBr in AcOH gave 28% N-(2,4,5-trichlorophenyl)-and 62% N-(4-bromo-2,5-dichlorophenyl)glycine, resp. The following new I were listed (Ar, % yield, and m.p. given): p-IC₆H₄, 50,

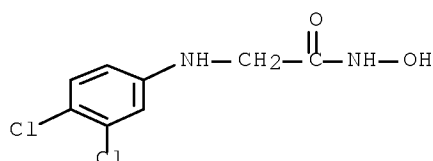
85-7°; 3-Cl-4-MeC₆H₃, 57, 91-3°; 3-Cl-4-MeOC₆H₃, 46, 110-12°; 3-I-4-MeOC₆H₃, 53, 109-10°; 2,5-Cl₂C₆H₃, 38, 30-1°; 3,4-Cl₂C₆H₃, 64, 104-6°; 2,3,4-Cl₃C₆H₂, 34, 61-3°; 2,4,5-Cl₃C₆H₂, 42, 77-8°; 3,4,5-Cl₃C₆H₂, 48, 135-7°; 2,5-Cl₂-4-BrC₆H₃, 54, 76-8°. Condensations of I with excess NH₂OH in MeOH containing 1 equivalent of NaOMe produced generally 75-85% ArNHCH₂C(=O)NH₂ (II), and were listed as follows (Ar and m.p. (decomposition) given): Ph, 117-18°; p-FC₆H₄, 111.5-12.0°; o-ClC₆H₄, 122.5-3.0°; m-ClC₆H₄, 107.5-8.0°; p-ClC₆H₄, 97.5-8.0° (decomposition); m-IC₆H₄, 116-6.5°; p-BrC₆H₄, 98-9°; p-IC₆H₄ (III), 107.5-8.0°; p-NO₂-C₆H₄, 132-3°; o-MeC₆H₄, 126.5-27°; m-MeC₆H₄, 109.5-10°; p-MeC₆H₄, 120.5-1.0°; o-EtC₆H₄, 104-5°; p-MeOC₆H₄, 136.5-7.5°; 2,4-F₂C₆H₃, 118.5-19.5°; 2,5-Cl₂C₆H₃, 136-7°; 3,4-Cl₂-C₆H₃, 110-11°; 3-Cl-4-MeC₆H₃, 117-18°; 3-Cl-4-MeOC₆H₃, 135-6°; 3-I-4-MeOC₆H₃, 149-9.5°; 2,3,4-Cl₃C₆H₂, 127.5-8.0°; 2,4,5-Cl₃C₆H₂, 122.5-3.0°; 3,4,5-Cl₃C₆H₂, 106-7.5°; 2,4-Cl₂-4-BrC₆H₂, 131.5-2.5°. III was the only compound of further interest as a herbicide, showing fungicidal activity with low phytotoxicity.

IT 14108-53-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14108-53-3 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]-N-hydroxy- (CA INDEX NAME)



L58 ANSWER 120 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:55413 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 66:55413

ORIGINAL REFERENCE NO.: 66:10463a,10466a

TITLE: N-Acylacridan derivatives

PATENT ASSIGNEE(S): Geigy, J. R., A.-G.

SOURCE: Neth. Appl., 18 pp.

CODEN: NAXXAN

DOCUMENT TYPE: Patent

LANGUAGE: Dutch

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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NL 6603820		19660926	NL 1966-3820	19660323
CH 455770			CH	
CH 455774			CH	
FR 1485593			FR	
FR 5626			FR	
GB 1137094			GB	
US 3452021		19690624	US	19660321
US 3498986		19700303	US	19680717
US 3498987		19700303	US	19680717
PRIORITY APPLN. INFO.:			CH	19650324

OTHER SOURCE(S): MARPAT 66:55413

GI For diagram(s), see printed CA Issue.

AB cf. preceding abstract The title compds. I are prepared Thus, 16.4 g. 10-(chloroacetyl)-9,9-dimethylacridan, 24 g. 3,4-dichlorobenzylamine and 0.1 g. KI in 100 cc. EtOH, refluxed 24 hrs. gave 10-[N-(3,4-dichlorobenzyl)glycyl]-9,9-dimethylacridan-HCl, m. 248°. Similarly were obtained the 10-derivs. HCl salts (m.p. given): [N-(2,4-dichlorobenzyl)glycyl], 285°; (N-benzylglycyl), 239°; [2,2-di(p-chlorophenyl)ethylglycyl], 246°; [N-(3-pyridyl)glycyl], 241°; [N-(5-chloro-2-pyridyl)glycyl], 180°; [N-(1-oxo-3-chlorobenzylamino)propyl], 208°; [N-(2,4-dichlorobenzyl)glycyl]-9-methylacridan, 230° and the analogous 3,4-dichlorobenzyl compound, 248°. From 10-(chloroacetyl)-9,9-dimethylacridan and 3,4-dichloroaniline was prepared 10-[N-(3,4-dichlorophenyl)glycyl]-9,9-dimethylacridan, m. 240°. Similarly were prepared the 10-derivs. (m.p. given): (N-phenylglycyl), 197°; [N-(p-chlorophenyl)glycyl], 216°; [N-(4-chloro- α,α,α -trifluoro-m-tolyl)glycyl], 166°; [N-(5-chloro(2-p-chlorophenoxy)phenyl)glycyl], 187°; [N-(o-biphenyl)glycyl], 174°; [N-(4,5-dichloro-o-toluy)glycyl], 212°; [N-(4-chloro-2,5-dimethoxyphenyl)glycyl], 174°; [N-(p-acetaminophenyl)glycyl], 245°; [N-(4-chloro-3-nitrophenyl)glycyl], 233°; [N-(m-aminophenyl)glycyl], 205°; [N-(2,4,5-trichlorophenyl)glycyl], 211°; 6-chloro-2-methoxy-10-[N-(3-trifluoromethyl-4-chlorophenyl)glycyl]-9,9-dimethylacridan, 202°; [N-(3,4-dichlorobenzyl)glycyl]-9,9-dimethyl-3-trifluoromethylacridan-HCl, 208°; and 10-[N-(3,4-dichlorophenyl)glycyl]-9,9-pentamethyleneacridan, 171°. From 10-(chloroacetyl)acridan (II), m. 120°, and PhNH₂ is prepared 10-(N-benzylglycyl)acridan-HCl, m. 215°; the analogous [N-(p-chlorobenzyl)glycyl]acridan-HCl, m. 220°. II and 3,4-dichloroaniline gave 10-[N-(3,4-dichlorophenyl)glycyl]acridan, m. 140°. Similarly were prepared I (R₁, R₂ = H) (m.p. given): (N-phenylglycyl), 167°; [N-(p-chlorophenyl)glycyl], 190°; [N-(2,4-dichlorophenyl)glycyl], 190°; [N-(5-chloro- α,α,α -trifluoro-m-tolyl)glycyl], 145°; [N-(3,4-xylyl)glycyl], 138°; [N-(α,α,α -trifluoro-m-tolyl)glycyl], 152°; [N-(3,4-dichlorophenyl)alanyl], 182°; [5-(3,4-dichlorobenzylamino)valeryl]-HCl, 157° (decomposition); [N-(3,4-dichlorophenyl)glycyl]-2-methylacridan, 142°; 10-(3-chloropropionyl)-9,9-dimethylacridan, 137-8° and p-chloroaniline gave 10-[N-(p-chlorophenyl)- β -alanyl]-9,9-dimethylacridan, 164°, HCl salt m. 192°. 10-[N-(2,4-dichlorobenzyl)-N-methylglycyl]-9,9-dimethylacridan-HCl, m. 204-5° (decomposition), 8.4 g. 9,9-dimethyl-10-(N-methylglycyl)acridan, m. 115°, 3.9 g. PhCH₂Cl, and 7.8 g. diisopropylethylamine, heated 20 hrs. to 140°, the product extracted with Et₂O-H₂O, the aqueous layer separated, the Et₂O solution washed with NaOH, the solvent evaporated, and the residue dissolved in Me₂CO and neutralized with (CO₂H)₂ gave 10-(N-benzyl-N-methylglycyl)-9,9-dimethylacridan-sesquioxalate, m. 190°. The compds. have antiviral and antitumor activity.

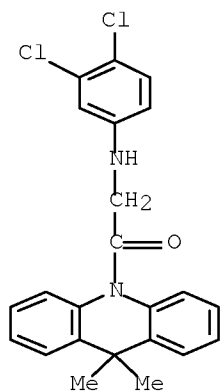
IT 13584-93-5P 13584-96-8P 13607-89-1P
13607-95-9P 13607-99-3P 13608-01-0P
13758-38-8P 13759-60-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13584-93-5 ZCAPLUS

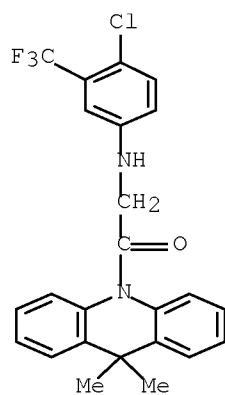
CN Acridan, 10-[N-(3,4-dichlorophenyl)glycyl]-9,9-dimethyl- (8CI) (CA INDEX NAME)

10/598508



RN 13584-96-8 ZCAPLUS

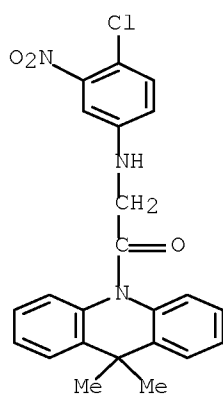
CN Acridan, 10-[N-(4-chloro- α,α,α -trifluoro-m-tolyl)glycyl]-
9,9-dimethyl- (8CI) (CA INDEX NAME)



RN 13607-89-1 ZCAPLUS

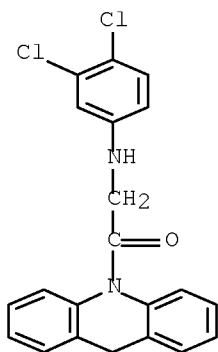
CN Acridan, 10-[N-(4-chloro-3-nitrophenyl)glycyl]-9,9-dimethyl- (8CI) (CA
INDEX NAME)

10/598508



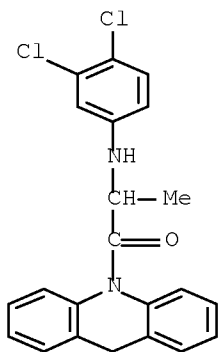
RN 13607-95-9 ZCAPLUS

CN Acridan, 10-[N-(3,4-dichlorophenyl)glycyl]- (8CI) (CA INDEX NAME)



RN 13607-99-3 ZCAPLUS

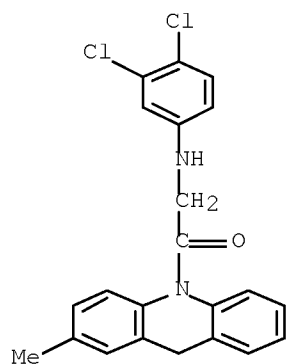
CN Acridan, 10-[N-(3,4-dichlorophenyl)alanyl]- (8CI) (CA INDEX NAME)



RN 13608-01-0 ZCAPLUS

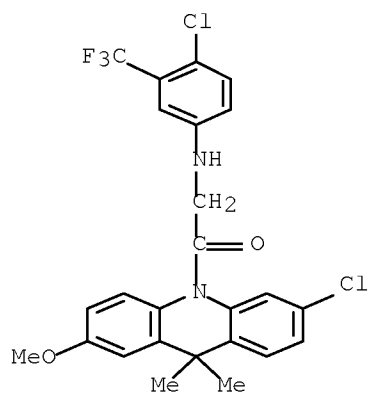
CN Acridan, 10-[N-(3,4-dichlorophenyl)glycyl]-2-methyl- (8CI) (CA INDEX NAME)

10/598508



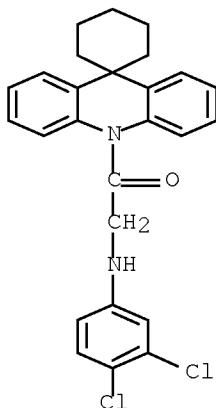
RN 13758-38-8 ZCAPLUS

CN Acridan, 6-chloro-10-[N-(4-chloro- α,α,α -trifluoro-m-tolyl)glycyl]-2-methoxy-9,9-dimethyl- (8CI) (CA INDEX NAME)



RN 13759-60-9 ZCAPLUS

CN Spiro[acridan-9,1'-cyclohexane], 10-[N-(3,4-dichlorophenyl)glycyl]- (8CI) (CA INDEX NAME)



L58 ANSWER 121 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1965:424440 ZCAPLUS Full-text

DOCUMENT NUMBER: 63:24440

ORIGINAL REFERENCE NO.: 63:4383e-g

TITLE: Aromatic fluorine compounds. XIII. Substituted N-phenylglycine ethyl esters and hydrazides

AUTHOR(S): Finger, G. C.; Dickerson, D. R.; Starr, L. D.; Orlopp, D. E.

CORPORATE SOURCE: Illinois State Geol. Surv., Urbana

SOURCE: Journal of Medicinal Chemistry (1965), 8(3), 405-7

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB cf. CA 61, 5561e. A large number of substituted N-phenylglycine Et esters (I) and hydrazides (II) were prepared as a part of program on the synthesis of fluorinated herbicides and medicinals. A mixture of 0.75 mole NaOAc.3H₂O, 50-75 ml. EtOH, 0.5 mole appropriate mono- or di-substituted aniline, and 0.5 mole ClCH₂CO₂Et refluxed and stirred 24-48 hrs. gave 25-50% I, which refluxed (22 hrs.) with 95% N₂H₄ in EtOH gave .apprx.95% II. A total of 31 I and 28 II were prepared, the substituent(s) on the Ph group comprising F, Cl, Br, iodine, CF₃, Me, and combinations of these groups in various positions.

IT 2344-98-1P, Glycine, N-(3-chloro-4-fluorophenyl)-, ethyl ester
 2345-00-8P, Glycine, N-(4-chloro-m-tolyl)-, ethyl ester
 2345-02-0P, Glycine, N-(4-bromo- α,α ,
 α -trifluoro-m-tolyl)-, ethyl ester 2345-03-1P, Glycine,
 N-(4-chloro- α,α,α -trifluoro-m-tolyl)-, ethyl ester
 2345-05-3P, Glycine, N-(α,α,α ,4-tetrafluoro-m-
 tolyl)-, ethyl ester 2351-01-1P, Glycine, N-(3,4-difluorophenyl)-
 , hydrazide 2370-44-7P, Glycine, N-(3-chloro-4-fluorophenyl)-,
 hydrazide 2370-45-8P, Glycine, N-(4-chloro-m-tolyl)-, hydrazide
 2370-50-5P, Glycine, N-(4-bromo- α,α ,
 α -trifluoro-m-tolyl)-, isopropylidenehydrazide 2445-88-7P,
 Glycine, N-(3,4-difluorophenyl)-, ethyl ester 2554-18-9P,
 Glycine, N-(4-chloro- α,α,α -trifluoro-m-tolyl)-,
 isopropylidenehydrazide

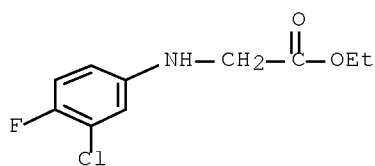
RL: PREP (Preparation)

(preparation of)

RN 2344-98-1 ZCAPLUS

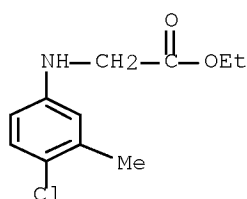
CN Glycine, N-(3-chloro-4-fluorophenyl)-, ethyl ester (CA INDEX NAME)

10/598508



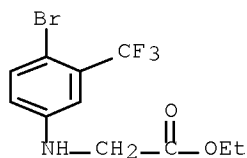
RN 2345-00-8 ZCAPLUS

CN Glycine, N-(4-chloro-m-tolyl)-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



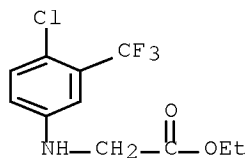
RN 2345-02-0 ZCAPLUS

CN Glycine, N-(4-bromo- α,α,α -trifluoro-m-tolyl)-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



RN 2345-03-1 ZCAPLUS

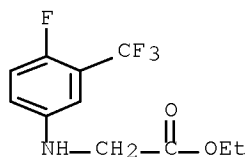
CN Glycine, N-[4-chloro-3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 2345-05-3 ZCAPLUS

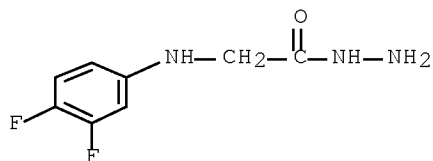
CN Glycine, N-(α,α,α ,4-tetrafluoro-m-tolyl)-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

10/598508



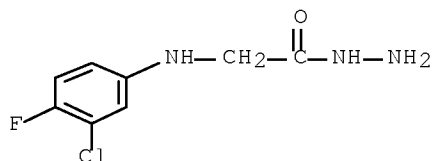
RN 2351-01-1 ZCAPLUS

CN Glycine, N-(3,4-difluorophenyl)-, hydrazide (CA INDEX NAME)



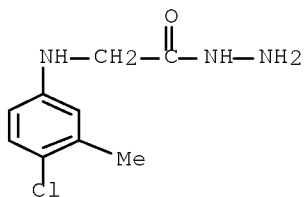
RN 2370-44-7 ZCAPLUS

CN Glycine, N-(3-chloro-4-fluorophenyl)-, hydrazide (CA INDEX NAME)



RN 2370-45-8 ZCAPLUS

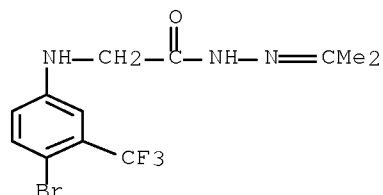
CN Glycine, N-(4-chloro-m-tolyl)-, hydrazide (7CI, 8CI) (CA INDEX NAME)



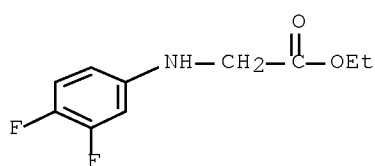
RN 2370-50-5 ZCAPLUS

CN Glycine, N-(4-bromo- α,α,α -trifluoro-m-tolyl)-, isopropylidenehydrazide (7CI, 8CI) (CA INDEX NAME)

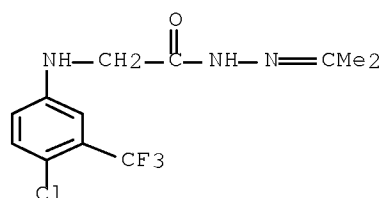
10/598508



RN 2445-88-7 ZCAPLUS
CN Glycine, N-(3,4-difluorophenyl)-, ethyl ester (CA INDEX NAME)



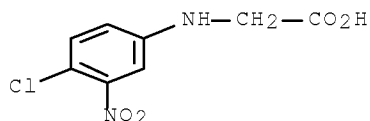
RN 2554-18-9 ZCAPLUS
CN Glycine, N-(4-chloro- α,α,α -trifluoro-m-tolyl)-, isopropylidenehydrazide (7CI, 8CI) (CA INDEX NAME)



L58 ANSWER 122 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:82248 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 60:82248
ORIGINAL REFERENCE NO.: 60:14345e-f
TITLE: SN Mechanism in aromatic compounds. XXX. Sydnone ring
AUTHOR(S): Chan, Tin-Lok; Miller, J.; Stansfield, F.
CORPORATE SOURCE: Univ. Hong Kong, Peop. Rep. China
SOURCE: Journal of the Chemical Society (1964), (Apr.),
1213-16
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 59, 4996a. The characteristics of the sydnone ring system have been investigated by making kinetic measurements with some 4-(R = substituted) 1-chloro-2-nitrobenzenes (including R = the sydnone ring), and comparing these

results with measurements on a suitable series of multiple-bond N groups. A close similarity to the β -azoxy grouping is demonstrated and discussed. The Hammett substituent constant (σ^*) for the p-N-sydnone ring is 0.710, compared with 0.769 for the p- β -azoxyphenyl group. Close similarity to the azido (or α -azoxyphenyl) group is not supported.

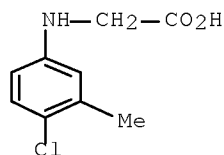
IT 89938-35-2P, Glycine, N-(4-chloro-3-nitrophenyl)-
 RL: PREP (Preparation)
 (preparation of)
 RN 89938-35-2 ZCAPLUS
 CN Glycine, N-(4-chloro-3-nitrophenyl)- (CA INDEX NAME)



L58 ANSWER 123 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1964:64041 ZCAPLUS Full-text
 DOCUMENT NUMBER: 60:64041
 ORIGINAL REFERENCE NO.: 60:11295h,11296e
 TITLE: Plant growth-regulating substances. XVII.
 Chloromethylphenoxyacetic acids and
 chloromethylphenylglycines
 AUTHOR(S): Clarke, G. G.; Wain, R. L.
 CORPORATE SOURCE: Wye Coll., London
 SOURCE: Annals of Applied Biology (1963), 51(3), 453-8
 CODEN: AABIAV; ISSN: 0003-4746
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB cf. *ibid.* 44, 547(1956). A number of substituted phenoxyacetic acids (I) were prepared by treating the appropriate Na phenolate with $\text{CH}_2\text{BrCO}_2\text{Et}$ and recrystg. the product from C_6H_6 . The corresponding phenylglycines (II) were prepared in 48-57% yield by refluxing for 4 h. a mixture of the appropriate aniline, $\text{CH}_2\text{ClCO}_2\text{H}$, and NaOAc in EtOH and recrystg. the product from C_6H_6 and (or) petr. ether. The substituent groups for I and II and their m.p., resp., were: 2-Cl-5-Me (III), 183-5° 201-4°; 2-Cl-4-Me (IV), 139-40°, 158-61°; 2-Cl-5-Me (V), 134.0-4.5, 128-9°; 2-Cl-6-Me (VI), 109-10° 180-1°; 3-Cl-2-Me, (VII), 164-5° 161-2.5°; 3-Cl-4-Me (VIII), 121-2.5°, 123-4°; 3-Cl-5-Me (IX), 80-1° 149-50.5°; 4-Cl-2-Me (X), 118-19°, 140-1°; 4-Cl-3-Me (XI), 177.5-8.5°, 115-16°; 5-Cl-2-Me (XII), 126-7°, 153-4°. The plant growth-regulating activity of all compds. was assessed in the wheat-cylinder, pea-segment, and pea-curvature tests. The order of activity for I in the wheat test was $\text{X} > \text{XI} > \text{XII} > \text{VII} > \text{V} > \text{III} = \text{IV} = \text{VI} = \text{VIII}$; IX was inactive in all 3 tests. The order of activity in the pea-segment and pea-curvature tests was $\text{X} > \text{XI} > \text{XII} = \text{VIII} > \text{VII} = \text{VI} = \text{IV} = \text{V} = \text{III}$; in the pea-curvature test, toxic effects were produced with the III and IX acids at 100 p.p.m. With II, the XI derivative showed activities comparable with the X acid in all 3 tests. In general, the II were less active than the I, with the exception of the VIII derivative in the wheat test.

IT 90942-43-1, Glycine, N-(4-chloro-m-tolyl)-
 (as plant growth regulator)
 RN 90942-43-1 ZCAPLUS
 CN Glycine, N-(4-chloro-m-tolyl)- (6CI, 7CI) (CA INDEX NAME)



L58 ANSWER 124 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1960:103125 ZCAPLUS Full-text

DOCUMENT NUMBER: 54:103125

ORIGINAL REFERENCE NO.: 54:19548b-f

TITLE: Synthesis of plant growth substances. IV.

α -(3,4-Dichloroanilino) fatty acids

AUTHOR(S): Wada, Hijiri; Takeda, Akira

SOURCE: Nogaku Kenkyu (1959), 47, 111-13

CODEN: NOGKAV; ISSN: 0029-0874

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 51, 8026e. Studies were made to test the effect of a Me radical in the α -position of 3,4-dichloro derivs. of N-arylglycine on their activities as plant growth substances. 3,4-Dichloroaniline (I) (16.2 g.) was refluxed in 40 ml. 3M NaHSO₃ in AcH, heating continued 10 min., after the mixture became clear, cooled, the resulting crystals dissolved in 40 ml. H₂O by warming, 9.1 g. KCN in 6 ml. H₂O added, the mixture warmed in boiling water about 1 hr., cooled, and filtered to obtain 17.9 g. α -(3,4-dichloroanilino)propionitrile (II), m. 115-16° (EtOH). II (10.8 g.) poured into 25 g. H₂SO₄ with vigorous agitation and with ice-cooling to keep the reaction temperature below 10°, warmed at 50-60° 30 min., and neutralized with 21 g. NaOH in 25 ml. H₂O gave 5.8 g. α -(3,4-dichloroanilino)propionamide (III), needles, m. 144-6° (decomposition) (hot H₂O). The crude preparation of III (4.7 g.) refluxed with 15 ml. 5% NaOH 2 hrs. more after the mixture became clear, diluted with 100 ml. H₂O, filtered, and adjusted pH to 3.0-3.5 with HCl precipitated 4.2 g. α -(3,4-dichloroanilino)propionic acid (IV), m. 146-8° (decomposition) (EtOH). I.HCl (19.8 g.), 6.5 g. KCN, and 11.6 g. Me₂CO boiled 20 min. with occasional shaking, 10 ml. H₂O added, boiling continued 1.5 hrs., the mixture cooled, and the precipitate crystallized from EtOH gave 14 g. α -(3,4-dichloroanilino)isobutyronitrile (V), m. 110-11° (EtOH). V (11.5 g.) poured into 25 g. H₂SO₄ below 30°, kept at 50-60° 1 hr., diluted with 25 ml. H₂O, and neutralized with 21 g. NaOH in 20 ml. H₂O gave 7.9 g. α -(3,4-dichloroanilino)isobutyramide (VI), needles, m. 146-7.5° (browning and decomposition) (hot H₂O). VI (6.2 g.) boiled with 40 ml. 20% NaOH 6 hrs., diluted with 100 ml. H₂O, filtered, and the pH adjusted to <3.0 with dilute HCl gave 4 g. α -(3,4-dichloroanilino)isobutyric acid (VII), m. 143-5° (browning and decomposition) (EtOH). Avena test and pea test showed that the plant growth activity of these compds. was less than that of N-(3,4-dichlorophenyl)glycine. Free acids IV and VII showed somewhat higher activity than their amides, III and VI. It was very interesting that VII and VI, in which both H atoms in α -position were substituted, showed the plant growth activity.

IT 28354-35-0P, Propionitrile, 2-(3,4-dichloroanilino)-

99282-71-0P, Propionamide, 2-(3,4-dichloroanilino)-

99421-37-1P, Propionitrile, 2-(3,4-dichloroanilino)-2-methyl-

103038-71-7P, Alanine, N-(3,4-dichlorophenyl)-2-methyl-

103505-36-8P, Propionamide, 2-(3,4-dichloroanilino)-2-methyl-

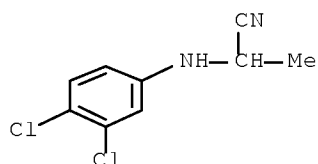
10/598508

RL: PREP (Preparation)

(preparation of)

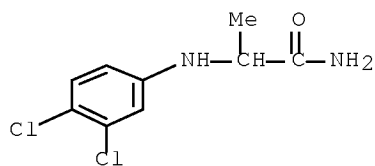
RN 28354-35-0 ZCAPLUS

CN Propanenitrile, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



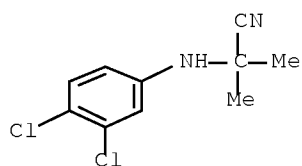
RN 99282-71-0 ZCAPLUS

CN Propionamide, 2-(3,4-dichloroanilino)- (6CI) (CA INDEX NAME)



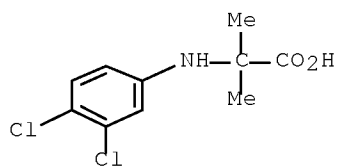
RN 99421-37-1 ZCAPLUS

CN Propionitrile, 2-(3,4-dichloroanilino)-2-methyl- (6CI) (CA INDEX NAME)



RN 103038-71-7 ZCAPLUS

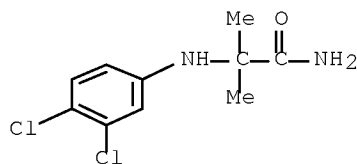
CN Alanine, N-(3,4-dichlorophenyl)-2-methyl- (CA INDEX NAME)



10/598508

RN 103505-36-8 ZCAPLUS

CN Propionamide, 2-(3,4-dichloroanilino)-2-methyl- (6CI) (CA INDEX NAME)



L58 ANSWER 125 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1959:115148 ZCAPLUS Full-text

DOCUMENT NUMBER: 53:115148

ORIGINAL REFERENCE NO.: 53:20641e-i

TITLE: m-Nitro- and m-trifluoromethylaryl acids as plant growth regulators

AUTHOR(S): Takeda, Akira

SOURCE: Contributions from Boyce Thompson Institute (1959), 20, 191-6

CODEN: CBTIAE; ISSN: 0006-8543

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB -A mixture of 49 g. (0.25 mole) of 3-trifluoromethyl-4-chloroaniline and 125 ml. of 3M formaldehyde-Na bisulfite solution refluxed for 1 hr. gave (3-trifluoromethyl-4-chlorophenylamino)methanesulfonate. The product dissolved in 125 ml. H₂O, mixed with 20 g. KCN in 50 ml. H₂O, refluxed for 1 hr. gave N-(3-trifluoromethyl-4-chlorophenyl)glycinonitrile, m. 76-8°. To prepare the amide: Add 4.7 g. (0.02 mole) of the nitrile to 6 ml. of concentrated H₂SO₄ (temperature kept below 30°). Warm the mixture to 60° for several min.; keep at room temperature for 3 min.; dilute with 100 ml. of H₂O with cooling; and neutralize with 20% aqueous NaOH. A yield of 2.1 g. of the amide, m. 109-111°, was obtained. To prepare the arylglycine: Heat 11.7 g. (0.05 mole) of the nitrile and 30 ml. concentrated HCl on a steam bath for 2 hrs., neutralize the mixture with 20% NaOH, dilute with 500 ml. of H₂O, adjust the pH to 6.0, clear with Norit, and acidify to below pH 4.0 with 1:1 HCl. A yield of 8.5 g., m. 130-1°, was obtained. Other new N-aryl glycines mentioned below were prepared similarly. The following compds. were active in the tomato-leaf epinasty test, N-(3,4-dichlorophenyl)glycine and its amide, N-(m-nitrophenyl)glycine and its amide, (m. 163-50°), m-nitrophenylacetic acid, m-nitrophenoxyacetic acid, N-(m-trifluoromethylphenyl)glycine, N-(3-trifluoromethyl-4-chlorophenyl)glycine (decomposition 130-1°) and its amide (m. 109-11°), m-(trifluoromethyl)phenoxyacetic acid. The following were active only when applied to the soil: N-(m-nitrophenyl)-N-methylglycinamide (m. 160-1°), m-nitrophenoxyacetamide, and α-(m-nitrophenoxy)propionic acid. N-(3-trifluoromethyl-4-chlorophenyl)glycinonitrile (m. 76-8°), 3,5-dinitrophenoxyacetic acid, and m-carboxyphenoxyacetic acid were inactive. The results show that when either the trifluoromethyl or the nitro group are present in the meta position of the benzene ring, there is an enhancement of activity. No enhancement of activity occurred when there was a carboxyl group in the meta position.

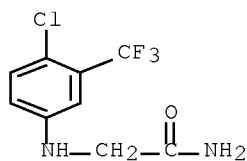
IT 721-32-4P, Acetamide, 2-(4-chloro-α,α,α-trifluoro-m-toluidino)- 782-61-6P, Glycine, N-(4-chloro-α,α,α-trifluoro-m-tolyl)- 2003-13-6P,

10/598508

Glycinonitrile, N-(4-chloro- α,α,α -trifluoro-m-tolyl)-
117919-59-2P, Acetamide, 2-(3,4-dichloroanilino)-
RL: PREP (Preparation)
(preparation of)

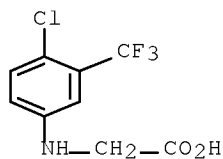
RN 721-32-4 ZCAPLUS

CN Acetamide, 2-[[4-chloro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



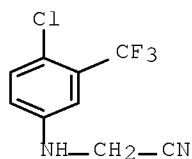
RN 782-61-6 ZCAPLUS

CN Glycine, N-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



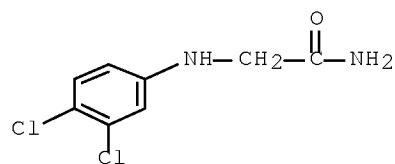
RN 2003-13-6 ZCAPLUS

CN Acetonitrile, (4-chloro- α,α,α -trifluoro-m-toluidino)-
(8CI) (CA INDEX NAME)



RN 117919-59-2 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 126 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:40336 ZCAPLUS Full-text

DOCUMENT NUMBER: 52:40336

ORIGINAL REFERENCE NO.: 52:7182e-g

TITLE: Possible plant hormones. I

AUTHOR(S): Sattur, N. B.; Kulkarni, S. N.; Nargund, K. S.

CORPORATE SOURCE: Karnatak Univ., Dharwar, India

SOURCE: Journal of the Karnatak University (1956), 1, 51-5

CODEN: JKAUAR; ISSN: 0453-3348

DOCUMENT TYPE: Journal

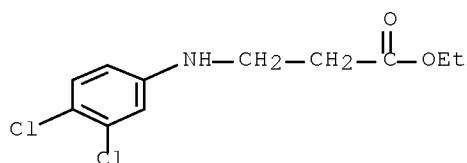
LANGUAGE: Unavailable

AB A series of aryl halo phenylglycine esters is described. These are lower homologs of γ -anilinobutyric acid, which is considered as a seco derivative of indoleacetic acid. Aryl halo anilines in 50% HOAc, containing NaOAc and ClCH₂CO₂H or Cl(CH₂)₂CO₂H were treated to form the amino acid derivs., characterized also as the Me and Et esters: 2,5-dichlorophenylglycine, m. 164-5°, Me ester, m. 52-3°, Et ester, b₆ 174°, n_{24D} 1.5535, d₃₁ 1.315; 2,4-dichlorophenylglycine, m. 152-3° (previously reported as 127°), Me ester, m. 58-9°, Et ester, m. 38-9°; 3,4-dichlorophenylglycine, m. 141-2°, Me ester, m. 109-10°, Et ester, m. 104°; 2,4,5-trichlorophenylglycine, m. 192-3°, Me ester, m. 110°, Et ester, m. 82°; 2-methyl-4-chlorophenylglycine, m. 147°, Me ester, m. 52°, Et ester, b₂₅ 290°; N-(2,5-dichlorophenyl)- β -alanine, m. 119-20°, Me ester, m. 59-60°, Et ester, m. 54-6°; N-(2,4-dichlorophenyl)- β -alanine, m. 98-9°, Me ester, b₁₈ 199-200°, n_{24D} 1.5595, d₃₁ 1.332, Et ester, b₁₅ 150-5°, n_{24D} 1.549, d₃₄ 1.294; N-(3,4-dichlorophenyl)- β -alanine, m. 132°, Me ester, m. 78°, Et ester, m. 71-2°; N-(2-methyl-4-chlorophenyl)- β -alanine, m. 82°, Me ester, b₈ 185°, n_{24D} 1.547, d₃₁ 1.212, Et ester, b₇ 189-90°, n_{24D} 1.537, d₃₁ 1.174.

IT 83442-84-6 99586-03-5 103038-72-8

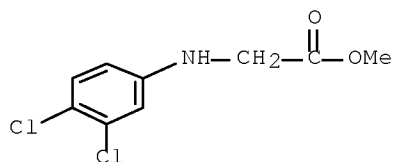
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 83442-84-6 ZCAPLUS

CN β -Alanine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

RN 99586-03-5 ZCAPLUS

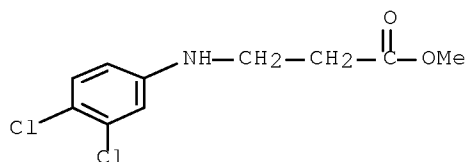
CN Glycine, N-(3,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)



10/598508

RN 103038-72-8 ZCAPLUS

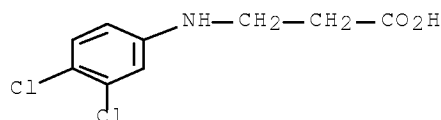
CN β -Alanine, N-(3,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)



IT 31399-32-3, β -Alanine, N-[3,4-dichlorophenyl]-
(and esters)

RN 31399-32-3 ZCAPLUS

CN β -Alanine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)



L58 ANSWER 127 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:29791 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 52:29791

ORIGINAL REFERENCE NO.: 52:5319h-i, 5320a-i, 5321a-b

TITLE: Synthesis of ring-substituted N-phenylglycines, their nitriles, and amides

AUTHOR(S): Takeda, Akira

CORPORATE SOURCE: Okayama, Univ., Kurasiki

SOURCE: Journal of Organic Chemistry (1957), 22, 1096-1100

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 52:29791

AB A series of 14 new 2,4-, 3,4-, and 2,4,5-substituted N-phenylglycines (I), RR'R''C₆H₂NHCH₂CO₂H, was synthesized from the corresponding arylamine (II), RR'R''HC₆H₂NH₂, through the Na N-arylaminomethanesulfonate (III), RR'R''C₆H₂NHCH₂SO₃Na, N-arylglycinonitrile (IV), RR'R''C₆H₂NHCH₂CN, and N-arylglycinamide (V), RR'R''C₆H₂NHCH₂CONH₂. Preliminary biol. testing by the Went pea test (C.A. 29, 22047) indicated that all I and V were active as plant growth substances. NaHSO₃ (375 g.) in 600 ml. H₂O stirred with gradual addition of 243 g. com. 37% HCHO and the mixture refluxed 10 min., filtered, and the filtrate made up to 1 l. with H₂O gave 3M HCHO-NaHSO₃ (VI). Br (32 g.) added slowly with stirring in 10 min. with rise of temperature to 60° to 36.6 g. 3,4-ClMeC₆H₃NHAc in 100 ml. AcOH and the mixture stirred 40 min. at 50-60°, poured slowly into 2 l. cold H₂O containing 6 g. NaHSO₃, and filtered yielded 47 g. 2,4,5-BrMeClC₆H₂NHAc, m. 153-4°(alc.), saponified with 20% NaOH to give pure II (R = Br, R' = Me, R'' = Cl) (VIa), m. 91-2° (alc.), deaminated to colorless material, b₄₀ 116-19°, oxidized with excess KMnO₄ in alkaline

solution to authentic 2,5-ClBrC₆H₃CO₂H, m. 157-8°. All tabulated compds. were prepared by essentially the procedures illustrated in the following detailed preps. VI (100 ml.) and 28.2 g. II (R = H, R' = Me, R'' = Cl) (VIb) refluxed 25 min. and the clear solution steam-distilled, the cooled distilland filtered, and the residue washed twice with 50 ml. alc. gave 47 g. methanesulfonate (VIc). KCN (7.2 g.) in 20 ml. H₂O added to 25.7 g. VIc in 50 ml. hot H₂O and the mixture refluxed 40 min., the cooled mixture filtered, and the product dried several days at room temperature in vacuo and 1 day at 40° gave IV (R = H, R' = Me, R'' = Cl) (VId), m. 62-3° (alc.). VIb (28.2 g.) in 40 ml. alc. stirred vigorously with 13.5 g. KCN in 35 ml. H₂O and 1 g. 30% aqueous KOH and the mixture refluxed 6 hrs. with stirring and addition of 16.2 g. 37% HCO, the mixture steam-distilled to recover 5.1 g. unreacted VIb and the distilland concentrated to 50 ml. on a steam bath, the concentrate treated with active C and filtered, the cooled filtrate adjusted to pH 4.0 with 1:1 HCl-H₂O and the mixture stored several hrs., filtered with suction, and the residue dried 12 hrs. at 60° gave 19.5 g. I (R = H, R' = Me, R'' = Cl) (VIE), m. 125-6° (decomposition) (dilute alc.) (method A). VId (3.6 g.) refluxed 3 hrs. with 60 ml. 5% aqueous NaOH and the cooled hydrolyzate filtered gave 0.3 g. V (R = H, R' = Me, R'' = Cl) (VIf), m. 152-3°. Treatment of the filtrate by concentration and acidification as above yielded 86% VIE (method B). VId (3.6 g.) and 60 ml. 1% aqueous NaOH stirred vigorously several min. at 94-5° until NH₃ was evolved, heating continued 20 min. and the cooled solution filtered, the impure product repeatedly extracted with 20 ml. hot H₂O and the white needles (2.6 g.) recrystd. from dilute alc. yielded VIf. Acidification of the filtrate gave 20% VIE. Cautious addition of a small excess of NH₄Et₂ to I in alc. and recrystn. from 1:1 EtOH-NH₄Et₂, gave analytically pure diethylamine salts (VII) of I. The properties and yields of I, VII, III, IV and V with their responses to the Went pea test (C.A. 29, 22047) were tabulated [I (R, R', R''), pH at which I were precipitated, m.p. (decomposition), % yields by methods A and B with % recovered II in parentheses, m.p. VII, and threshold min. concns. in mg./l. exhibiting activity in pea test given]: Cl, Cl, H, 5.2-5.4, 151-2°, 72(33), 87(-), 88-90°, 1.90; H, Cl, Cl, 5.2-5.4, 128-9°, 83(25), 82(7), 137-8°, 0.23; H, Cl, Me, 4.2-4.4, 125-6°, 60(18), 86(8), 120-1°, 6.02; H, Me, Cl, 4.2-4.4, 115-17°, -(-), 69(6), 134-4.5°, 3-22; Br, Me, H, 6.5-5.8, 169-70°, 54(66), 78(8), 123-4°, 6.30; Me, Br, H, 4.8-5, 142-5°, -(-), 82(6), 109-11°, 10.70; Cl, Me, H, 4.2-4.6, 161-4°, 31(71), 91(-), 110-11°, 20.20; Me, Cl, H, 4.2-4.4, 143-4°, 57(52), 83(5), 109-10°, 7.30; Cl, Br, H, 5.6-5.8, 156-7°, -(-), 90(3), 107-8°, 4.20; Br, Cl, H, 5.6-5.8, 163-4°, -(-), 87(6), 118-18.5°, 5.02; Cl, Cl, Cl, 4-4.2, 185-6°, 89(54), 62(8), 174-5°, 0.35; Cl, Me, Cl, 4.6-4.8, 173-5°, -(-), 83(4), 141-3°, 14.50; Br, Me, Cl, 6.2-6.4, 195-6°, -(-), 85(4), 170-4°, 14.70; H, Me, NO₂, 3.8-4.2, 147-9°, -(-), 82(6), 149-50°, 4.52; H, Cl, NO₂, 3.8-4, 174.5-5°, -(-), 67(17), 128-9°, 0.79. [III (R, R', R''), reaction time in min., and % yield on consumed I with % recovered I in parentheses given]: Cl, Cl, H, 120, 87(23); H, Cl, Cl, 25, 94(0); H, Me, Cl, 25, 91(1); H, Cl, Me, 25, 90(0); Br, Me, H, 60, 88(7); Me, Br, H, 40, 99.5(0); Cl, Me, H, 120, 84(8); Me, Cl, H, 120, 90(16); Cl, Br, H, 120, 86(44); Br, Cl, H, 120, 69(51); Cl, Cl, Cl, 180, 38(84); Cl, Me, Cl, 180, 42(71); Br, Me, Cl, 180, 82(83); H, Me, NO₂, 20, 84(0); H, Cl, NO₂, 20, 87(0). [IV (R, R', R''), m.p., and % yield given]: Cl, Cl, H, 76-8°, 87; H, Cl, Cl, 101-2°, 95; H, Me, Cl, 62-3°, 91; H, Cl, Me, 86-7°, 83; Br, Me, H, 62-3°, 89; Me, Br, H, 104.5-5.5°, 89; Cl, Me, H, 47-8°, 83; Me, Cl, H, 101-1.5°, 86; Cl, Br, H, 81-2°, 90; Br, Cl, H, 104-5°, 94; Cl, Cl, Cl, 122-3°, 91; Cl, Me, Cl, 110-12°, 91; Br, Me, Cl, 121-2°, 74; H, Me, NO₂, 101-2°, 99; H, Cl, NO₂, 90.5-1.5°, 92. [V (R, R', R''), m.p. (decomposition), % yield and % IV converted to I in parentheses, and pea test activity given]: Cl, Cl, H, 141-2°, 27(5), 1.36; H, Cl, Cl, 139-9.5°, 49(37), 0.25; H, Me, Cl, 152-3°, 66(2), 4.55; H, Cl, Me, 122-3°, 38(36), 6.40; Br, Me, H, 149.5-50.5°,

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38(45), 10.80; Me, Br, H, 156-7°, 40(39), 20.20; Cl, Me, H, 134-5°, 18(55), 42.25; Me, Cl, H, 152.5-4°, 37(48), 3.86; Cl, Br, H, 150-1°, 46(45), 4.43; Br, Cl, H, 144-6°, 44(51), 2.85; Cl, Cl, Cl, 152-3°, 47(31), 0.27; Cl, Me, Cl, 156-7°, 55(24), 10.10; Br, Me, Cl, 167-8°, 44(40), -; H, Me, NO₂, 143.5-4°, 48(36), 5.18; H, Cl, NO₂, 141-2°, 48(33), 1.05. Neither of the Cl atoms in the most active I (R = H, R' = Cl, R'' = Cl) (VIIa) can be replaced by an Me group without loss of biol. activity whereas the o-Cl atom in I (R = Cl, R' = Cl, R'' = H) (VIIf) can be replaced. I (R = R' = R'' = Cl) is as active as VIIa and the replacement of the p-Cl atom in VIIf is accompanied by considerable decrease in biol. activity.

IT 108880-36-0 109726-01-4

(Derived from data in the 6th Collective Formula Index (1957-1961))

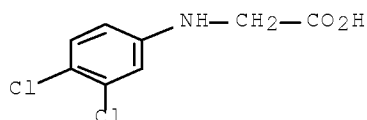
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CN Glycine, N-(3,4-dichlorophenyl)-, Et₂NH salt (6CI) (CA INDEX NAME)

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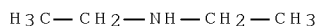
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CM 2

CRN 109-89-7

CMF C4 H11 N



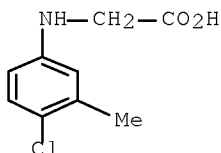
RN 109726-01-4 ZCAPLUS

CN Glycine, N-(4-chloro-m-tolyl)-, Et₂NH salt (6CI) (CA INDEX NAME)

CM 1

CRN 90942-43-1

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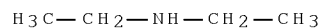


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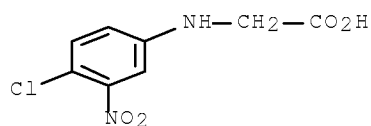
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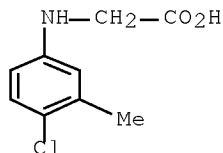
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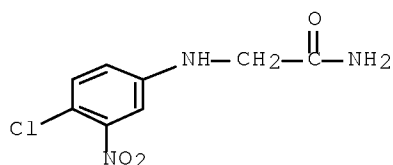
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Acetamide, 2-(4-chloro-3-nitroanilino)- 103037-86-1P, Acetamide,
2-[4-chloro-m-toluidino]- 109018-98-6P, Glycine,
N-(4-chloro-3-nitrophenyl)-, diethylamine salt 117069-73-5P,
Glycinonitrile, N-[4-chloro-m-tolyl]- 117887-53-3P,
Glycinonitrile, N-(4-chloro-3-nitrophenyl)- 117919-59-2P,
Acetamide, 2-[3,4-dichloroanilino]-
RL: PREP (Preparation)
(preparation of)
RN 89938-35-2 ZCAPLUS
CN Glycine, N-(4-chloro-3-nitrophenyl)- (CA INDEX NAME)



RN 90942-43-1 ZCAPLUS
CN Glycine, N-(4-chloro-m-tolyl)- (6CI, 7CI) (CA INDEX NAME)



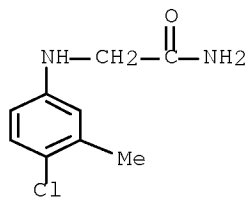
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CN Acetamide, 2-(4-chloro-3-nitroanilino)- (6CI) (CA INDEX NAME)



10/598508

RN 103037-86-1 ZCAPLUS

CN Acetamide, 2-(4-chloro-m-toluidino)- (6CI) (CA INDEX NAME)



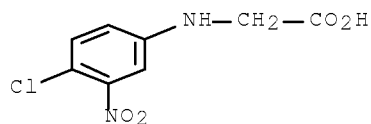
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CN Glycine, N-(4-chloro-3-nitrophenyl)-, Et2NH salt (6CI) (CA INDEX NAME)

CM 1

CRN 89938-35-2

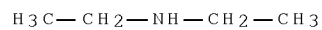
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CM 2

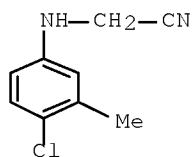
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CMF C4 H11 N



RN 117069-73-5 ZCAPLUS

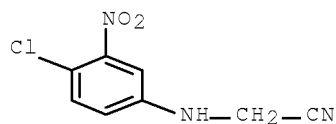
CN Glycinonitrile, N-(4-chloro-m-tolyl)- (6CI) (CA INDEX NAME)



10/598508

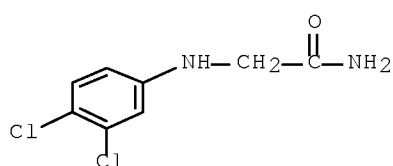
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CN Acetonitrile, [(4-chloro-3-nitrophenyl)amino]- (9CI) (CA INDEX NAME)



RN 117919-59-2 ZCAPLUS

CN Acetamide, 2-[(3,4-dichlorophenyl)amino]- (CA INDEX NAME)



L58 ANSWER 128 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:29790 ZCAPLUS Full-text

DOCUMENT NUMBER: 52:29790

ORIGINAL REFERENCE NO.: 52:5319h

TITLE: Hydrogen bond and properties of nitroanilines

AUTHOR(S): Lutskii, A. E.

SOURCE: Zhurnal Obshchei Khimii (1956), 26, 2567-70

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB See C.A. 51, 4976i.

IT 108880-36-0 109726-01-4

(Derived from data in the 6th Collective Formula Index (1957-1961))

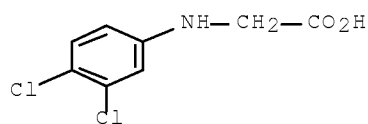
RN 108880-36-0 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)-, Et2NH salt (6CI) (CA INDEX NAME)

CM 1

CRN 65051-17-4

CMF C8 H7 Cl2 N O2



CM 2

10/598508

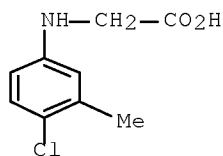
CRN 109-89-7
CMF C4 H11 N



RN 109726-01-4 ZCAPLUS
CN Glycine, N-(4-chloro-m-tolyl)-, Et2NH salt (6CI) (CA INDEX NAME)

CM 1

CRN 90942-43-1
CMF C9 H10 Cl N O2



CM 2

CRN 109-89-7
CMF C4 H11 N



L58 ANSWER 129 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1958:29789 ZCAPLUS Full-text
DOCUMENT NUMBER: 52:29789
ORIGINAL REFERENCE NO.: 52:5319f-h
TITLE: Synthesis of 2,5- and 3,5-dibromoanilines and 2,3,5- and 3,4,5-tribromoanilines
AUTHOR(S): Hayashi, Takayuki
CORPORATE SOURCE: Yamaguchi Univ.
SOURCE: Kogyo Kagaku Zasshi (1956), 59, 715-17
CODEN: KGKZA7; ISSN: 0368-5462
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 2,5-Br2C6H3NH2 was prepared from 2,5-Br2C6H3NO2 by reduction with Sn and HCl at 90°. Similarly, 3,5-Br2C6H3NH2 was obtained by reduction of 3,5-Br2C6H3NO2, which was prepared from diazotized 2,6,4-Br2(O2N)C6H2NH2 (I) by treating with EtOH and CuSO4. Reduction of 3,4,5-Br3C6H2NO2, which was obtained by Sandmeyer reaction of I, gave 3,4,5-Br3C6H2NH2. 2,3,5-Br3C6H2NH2

10/598508

was prepared from o-O₂NC₆H₄NH₂ through 2,4,6-Br₂(O₂N)C₆H₂NH₂ and 2,3,5-Br₃C₆H₂NO₂ (Sandmeyer reaction).

IT 108880-36-0 109726-01-4

(Derived from data in the 6th Collective Formula Index (1957-1961))

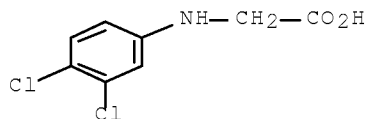
RN 108880-36-0 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)-, Et₂NH salt (6CI) (CA INDEX NAME)

CM 1

CRN 65051-17-4

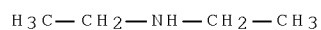
CMF C8 H7 Cl₂ N O₂



CM 2

CRN 109-89-7

CMF C₄ H₁₁ N



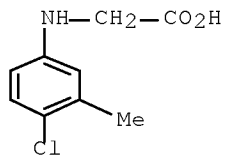
RN 109726-01-4 ZCAPLUS

CN Glycine, N-(4-chloro-m-tolyl)-, Et₂NH salt (6CI) (CA INDEX NAME)

CM 1

CRN 90942-43-1

CMF C₉ H₁₀ Cl N O₂



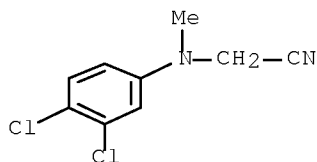
CM 2

CRN 109-89-7

CMF C₄ H₁₁ N



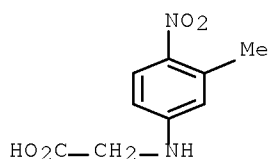
L58 ANSWER 130 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1957:43178 ZCAPLUS Full-text
 DOCUMENT NUMBER: 51:43178
 ORIGINAL REFERENCE NO.: 51:8026e-g
 TITLE: Synthesis of plant-growth substances. III.
 N-Methyl-N-phenylglycine derivatives
 AUTHOR(S): Takeda, Akira; Wada, Sei; Fujimoto, Munehiro
 CORPORATE SOURCE: Okayama Univ.
 SOURCE: Rept. Ohara Inst. Agr. Biol. (1956), 44, 98-104
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. C.A. 49, 11792i. 3,4-Cl₂C₆H₃NHMe (from 3,4-Cl₂C₆H₃NH₂ with Me₂SO₄ through the NMe₂ derivative and N(NO)Me derivative or from 3,4-Cl₂C₆H₃NHCH₂CO₂H decarboxylated by boiling) was boiled 5.5 hrs. with (CH₂O)₃ and NaHSO₃ to form 3,4-Cl₂C₆H₃NMeCH₂SO₃Na, then heated 30 min. near the b.p. with KCN to replace SO₃Na with CN, and finally saponified with concentrated H₂SO₄ at 50-60° 30 min. to 3,4-Cl₂C₆H₃NMeCH₂CONH₂ (I), needles, m. 166-8° (from hot H₂O). Similarly, from 4-ClC₆H₄NHMe was obtained 4-ClC₆H₄NMeCH₂CONH₂ (II), m. 133-5°. In the Adzuki bean, Went pea, and Avena cylinder tests, I and III were found less growth-promoting than each respective unmethylated phenylglycinamide.
 IT 109047-40-7P, Glycinonitrile, N-(3,4-dichlorophenyl)-N-methyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 109047-40-7 ZCAPLUS
 CN Glycinonitrile, N-(3,4-dichlorophenyl)-N-methyl- (6CI) (CA INDEX NAME)



L58 ANSWER 131 OF 131 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1915:13121 ZCAPLUS Full-text
 DOCUMENT NUMBER: 9:13121
 ORIGINAL REFERENCE NO.: 9:2063f-i,2064a-c
 TITLE: Nitrotolylglycine
 AUTHOR(S): Pollak, W.
 CORPORATE SOURCE: Vienna
 SOURCE: Journal fuer Praktische Chemie (Leipzig) (1915), 91, 285-306
 CODEN: JPCEAO; ISSN: 0021-8383
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB BrCH₂CO₂H reacts readily with 2,4- and 2,6-H₂N(O₂N)C₆H₃Me with the formation of the corresponding glycine derivs., but there is practically no reaction when ClCH₂CO₂H is used. 2,4-O₂N(H₂N)C₆H₃Me with the above AcOH derivs. yielded

mere traces of the glycine derivs. The reaction is expressed by the following equations: $3\text{C}_7\text{H}_6(\text{NO}_2)\text{NH}_2 + \text{BrCH}_2\text{CO}_2\text{H} = \text{CH}_2(\text{NHC}_7\text{H}_6\text{NO}_2)\text{CO}_2\text{H} \cdot \text{C}_7\text{H}_6(\text{NO}_2)\text{NH}_2(\text{a}) + \text{C}_7\text{H}_6(\text{NO}_2)\text{NH}_2 \cdot \text{HBr}$; $(\text{a}) + \text{NaOH} = \text{CH}_2(\text{NHC}_7\text{H}_6\text{NO}_2)\text{CO}_2\text{Na} + \text{C}_7\text{H}_6(\text{NO}_2)\text{NH}_2 + \text{H}_2\text{O}$. These glycine derivs. have strong acidic properties, dissolving readily in alkali carbonates. The following derivs. of 2,4-H₂N(O₂N)C₆H₃Me were prepared: on slowly heating 3 mols. amine with BrCH₂CO₂H up to 90°, the fused product suddenly solidified, at the same time changing from reddish to yellowish brown. Further heating for 3 hrs., then boiling with H₂O, making alkaline with NaOH, filtering off the H₂N(O₂N)C₆H₃Me and acidifying the filtrate with dilute HCl, gave 1,2,4-nitrotolylglycine (b) in 85% yield, lustrous, yellow needles from H₂O, m. 140°; silver salt, small needles, unstable in the air; copper salt, $[\text{C}_7\text{H}_6(\text{NO}_2)\text{NHCH}_2\text{CO}_2]_2\text{Cu} \cdot \text{H}_2\text{O}$, beautiful green crystals, m. 195°; methyl ester, from the Ag salt and MeI, yellow needles, m. 108°; ethyl ester, from alc. HCl, reddish brown needles, m. 42°; 1,2,4-aminotolylglycine hydrochloride, by reducing (b) with Zn dust and HCl, brown crystals from alc., m. 98°. Diazotized and coupled with alc. β-naphthol it gave a dye, and also a reddish brown dye with "R" salt: on heating for 4-5 hrs. at 150-60°, (b) gave 1,2,4-dinitroditolyl-α,γ-diacipiperazine, bright yellow compound by precipitating from AcOH with H₂O, m. 186°, insol. in alkalies. It is decomposed into its components by boiling with alc. KOH. In a similar way the following derivs. of 4,2-H₂N(O₂N)C₃H₃Me were prepared: 1,4,2-Nitrotolylglycine, yellow prisms from alc., m. 130°; ammonium salt, reddish brown prisms, m. 135°, which with (AcO)₂Pb forms the lead salt, microscopic orange needles; copper salt + H₂O, green crystals, m. 160°. From 2,6-H₂N(O₂N)C₆H₃Me the following derivs. were obtained: 1,2,6-Nitrotolylglycine, yellowish brown prisms from alc., m. 152°; silver salt, very unstable; lead salt + H₂O, grayish yellow compound, m. 170°. Somewhat similarly, 2,5- and 3,6-H₂N(O₂N)C₆H₃Me gave the following derivs.: 1,2,5-Nitrotolylglycine (c), reddish brown crystals from alc., m. 192°; on heating it does not yield a piperazine derivative; lead salt, yellow compound; barium salt + 0.5 H₂O, from the acid + BaCO₃, yellowish brown needles; NaNO₂ gives with (c) in dilute HCl the nitroso derivative, $\text{C}_7\text{H}_6(\text{NO}_2)\text{N}(\text{NO})\text{CH}_2\text{CO}_2\text{H}$, m. 110°; ethyl ester, from 2 mols. 2,5-H₂N(O₂N)C₆H₃Me and ClCH₂CO₂Et at 130-40° for 2 days, also by esterifying (c) with HCl, crystals from C₆H₆, m. 87°; methyl ester, from the Ag salt and MeI, yellow needles from C₆H₆, m. 82°; 1,3,6-nitrotolylglycine, yellow crystals from H₂O, m. 145°. It gives colored, crystalline salts with most of the bases.

IT 861570-09-4P, Glycine, N-(4-nitro-m-tolyl)-
 RL: PREP (Preparation)
 (preparation of)
 RN 861570-09-4 ZCAPLUS
 CN Glycine, N-(4-nitro-m-tolyl)- (1CI) (CA INDEX NAME)



10/598508

ACCESSION NUMBER: 1958:40336 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 52:40336
 ORIGINAL REFERENCE NO.: 52:7182e-g
 TITLE: Possible plant hormones. I
 AUTHOR(S): Sattur, N. B.; Kulkarni, S. N.; Nargund, K. S.
 CORPORATE SOURCE: Karnatak Univ., Dharwar, India
 SOURCE: Journal of the Karnatak University (1956), 1, 51-5
 CODEN: JKAUAR; ISSN: 0453-3348
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

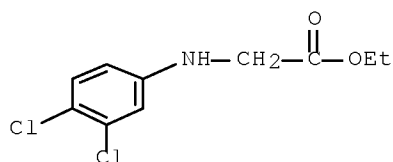
AB A series of aryl halo phenylglycine esters is described. These are lower homologs of γ -anilinobutyric acid, which is considered as a seco derivative of indoleacetic acid. Aryl halo anilines in 50% HOAc, containing NaOAc and ClCH₂CO₂H or Cl(CH₂)₂CO₂H were treated to form the amino acid derivs., characterized also as the Me and Et esters: 2,5- dichlorophenylglycine, m. 164-5°, Me ester, m. 52-3°, Et ester, b6 174°, n₂₄D 1.5535, d₃₁ 1.315; 2,4- dichlorophenylglycine, m. 152-3° (previously reported as 127°), Me ester, m. 58-9°, Et ester, m. 38-9°; 3,4-dichlorophenylglycine, m. 141-2°, Me ester, m. 109-10°, Et ester, m. 104°; 2,4,5-trichlorophenylglycine, m. 192-3°, Me ester, m. 110°, Et ester, m. 82°; 2-methyl-4-chlorophenylglycine, m. 147°, Me ester, m. 52°, Et ester, b₂₅ 290°; N-(2,5-dichlorophenyl)- β -alanine, m. 119-20°, Me ester, m. 59-60°, Et ester, m. 54-6°; N-(2,4-dichlorophenyl)- β -alanine, m. 98-9°, Me ester, b₁₈ 199-200°, n₂₄D 1.5595, d₃₁ 1.332, Et ester, b₁₅ 150-5°, n₂₄D 1.549, d₃₄ 1.294; N-(3,4-dichlorophenyl)- β - alanine, m. 132°, Me ester, m. 78°, Et ester, m. 71-2°; N-(2-methyl-4-chlorophenyl)- β -alanine, m. 82°, Me ester, b₈ 185°, n₂₄D 1.547, d₃₁ 1.212, Et ester, b₇ 189-90°, n₂₄D 1.537, d₃₁ 1.174.

IT 14108-81-7

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 14108-81-7 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)



L65 ANSWER 16 OF 16 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1955:61248 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 49:61248
 ORIGINAL REFERENCE NO.: 49:11793a-c
 TITLE: Synthesis of plant-growth substances. II.
 Phenylglycine derivatives (1)
 AUTHOR(S): Takeda, Akira
 CORPORATE SOURCE: Okayama Univ.
 SOURCE: Nogaku Kenkyu (1954), 42, 19-48
 CODEN: NOGKAV; ISSN: 0029-0874
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

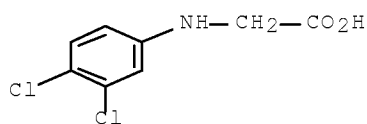
10/598508

AB As tested with peas and adsuki (*Phaseolus angularis*) beans, PhNHCH₂CO₂H (I) and its substitutions at the N were all active except the Ac derivative, proving generally that the activity is not affected by linking a side-chain carboxyalkyl radical with an aromatic nucleus through NH any more than linking through O or S. Unlike substituted PhOCH₂CO₂H or CH(Ph)SHCO₂H, however, the m-substitutions were more active here than the o-substitutions. 3,4-C₁₂C₆H₃NHCH₂CO₂H was about equally active as 1-C₁₀H₇OAc or (2,4-C₁₂C₆H₃O)OAc, but 2,4-C₁₂C₆H₃NHCH₂CO₂H was slightly less so. 4-C₁C₆H₄NHCH₂CO₂H lost no activity by carboxymethylation at the N, but lost the accelerating power of cellular elongation by acetylation. However, it showed only pos. curvature in the adsuki bean test and affected further growth due either to its direct action or to substituted I hydrolyzed from a plant tissue at a carbamide linkage by an enzymic action. In substituted I, CO₂H could not be replaced by -SO₃H.

IT 65051-17-4, Glycine, N-[3,4-dichlorophenyl]-
(plant-growth-promoting activity of)

RN 65051-17-4 ZCAPLUS

CN Glycine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)



L66 ANSWER 15 OF 15 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:506282 ZCAPLUS Full-text

DOCUMENT NUMBER: 69:106282

ORIGINAL REFERENCE NO.: 69:19887a,19890a

TITLE: Wild oat herbicides

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij N. V.

SOURCE: Neth. Appl., 20 pp.
CODEN: NAXXAN

DOCUMENT TYPE: Patent

LANGUAGE: Dutch

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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NL 6717715	A	19680701	NL 1967-17715	19671228
GB 1164160	A	19690917	GB 1966-58406	19661230
FR 1575558	A	19690725	FR 1967-1575558	19671228
CH 498087	A	19701031	CH 1967-498087	19671228
DK 123025	B	19720508	DK 1967-6557	19671228
DE 1643527	C3	19791011	DE 1967-S113544	19671228
DE 1643527	B2	19790222		

PRIORITY APPLN. INFO.: GB 1966-58406 A 19661230

GI For diagram(s), see printed CA Issue.

AB Title compds. (I) were prepared from the corresponding II. Thus, 500 cc. water and 3600 g. 2-chloropropionic acid were added to a solution of 2686 g. 3,4-dichloroaniline in 8400 cc. iso-PrOH. The mixture was heated to 40°, 5600

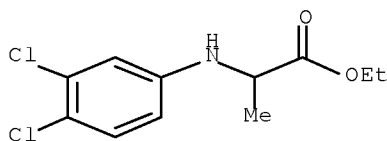
g. NaHCO₃ added, and the mixture refluxed 113 hrs., cooled, poured into 100 l. water, filtered, acidified with HCl to pH 3-4, and filtered. The precipitate was washed and dried to give 2455 g. N-(3,4-dichlorophenyl)alanine (III), m. 148-9°. A solution of 2475 g. III in 10 l. absolute EtOH was refluxed 6 hrs., while passing gaseous HCl, and kept overnight to give 2176 g. II (R₁ = R₂ = Cl, R₃ = R₅ = H, n = 2, Y = CO₂Et) (IV), m. 37-8°. IV refluxed 4 hrs. with 1450 g. BzCl in anhydrous benzene, and another 20 hrs. with 290 g. addnl. BzCl to give 2220 g. I (R₁ = R₂ = Cl, R₃ = R₅ = H, R₄ = Ph, n = 2, Y = CO₂Et), m. 50-2°. Similarly prepared were the following I (R₁ = R₂ = Cl, R₃ = R₅ = H, Y = CO₂Et) (R₄, n, and n₂1D given): Me, 2, 1.5383 (b₀·4 147-8°); Et₂O 2, 1.5271 (b₀·35 150°); Et, 2, 1.5307; 2,4-MeClC₆H₃OCH₂, 2, 1.5650; Ph, 1, 1.5734; cyclopropyl, 2, 1.5430; p-MeC₆H₄, 2, - (m. 55-60°); p-O₂NC₆H₄, 2, 1.5740; m-ClC₆H₄, 2, -. Also prepared were the following I (R₄ = Ph, R₅ = H, n = 2, Y = CO₂Et) (R₁, R₂, R₃, and n₂1D given): Cl, H, H, 1.5620; H, Cl, H, 1.5588; H, H, H, 1.5536; Cl, H, Me, 1.5506; Bu, H, H, 1.5373; Cl, H, MeO, - (m. 129-31°); Cl, CF₃, H, -. Also prepared are the following I (R₁, R₂, R₃, R₄, R₅, n, Y, and m.p. given): Cl, Cl, H, Ph, H, 2, CO₂H, 155-7°; Cl, Cl, H, Ph, Me, 1, CONHMe, 163-5°; Cl, H, H, Ph, H, 2, CO₂H, 152-3°; Me, Cl, H, Ph, Me, 1, CONHMe, 146-7°; NO₂, NO₂, H, p-ClC₆H₄, H, 2, CO₂Et, -. I are used to protect cereal grains against wild oats.

IT 22212-58-4F

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 22212-58-4 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)



L67 ANSWER 14 OF 14 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1955:9719 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 49:9719

ORIGINAL REFERENCE NO.: 49:2000g-i,2001a-e

TITLE: Note on a method for the estimation of exchangeable bases in black soils containing free calcium carbonate and soluble salts including gypsum

AUTHOR(S): Menon, P. K. R.; Sankaranarayanan, M. P.

SOURCE: Madras Agricultural Journal (1953), 40, 43-46

CODEN: MAAJAP; ISSN: 0024-9602

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB In crop rotation on calcareous soils, cotton following cholam was stunted in growth. The yield was also less as compared with cotton following cumbu. This harmful effect of cholam on cotton is being investigated. To ascertain if an increase of Na in the soil is the cause, exchangeable Na had to be determined. Since there was no satisfactory method, 2 new procedures were evolved. Procedure for calcareous soils and alkaline soils not containing gypsum: Ten g. of the air-dried soil is weighed out into a beaker to which is

added with stirring 50 cc. of 40% EtOH adjusted to pH 7.05 with NH₄OH. The solution is allowed to stand, and the clear supernatant liquid is transferred to a filter. The soil is washed by decantation 3 times for calcareous soils not containing much of soluble salts, especially sulfate in the form of gypsum. The washed soil is leached in the cold with 500 cc. of 0.5N NH₄OAc solution adjusted to pH 8.4 with NH₄OH. The leachate is evaporated to about 100 cc., and Ca is estimated in it as Ca oxalate by a volumetric method. The filtrate and washings from the Ca estimation are evaporated to dryness on a water bath after the addition of about 1 cc. of 1:1 H₂SO₄. The residue is ignited to remove NH₄ salts and then dissolved in dilute HCl and made up to 250 cc. In 75-cc. aliquots the following were determined: Mg as Mg₂P₂O₇, Na as Na uranyl Mg acetate, and K as the K₂PtCl₆ or K cobaltinitrite. The leached soil is saturated with 10 cc. of 0.5N NH₄Cl solution and then washed with 40% EtOH adjusted to pH 7.0 until the washings run free from chloride. The washed ammonium soil is distilled with MgO, and the NH₃ liberated is estimated to obtain the base-exchange capacity of the soil. Procedure for calcareous soils containing gypsum: In the case of such soils after washing 3 to 6 times with 40% EtOH 10 g. of the soil is digested with 20 cc. of saturated Ba(OH)₂ solution, stirred vigorously, and allowed to stand for 0.5 hr. with frequent stirring. CO₂ is bubbled through the mixture to precipitate the excess of Ba as BaCO₃. The mixture is then heated on a water bath at about 80° for about 15 min. To the soil 100 cc. of 0.5N NH₄OAc adjusted to pH 7.0 is added, and the mixture allowed to stand at about 60° for 0.5 hr. The mixture is filtered and washed by decantation 3 times with 50-cc. portions of 0.5N NH₄OAc. The soil is transferred completely to the filter and leached with NH₄OAc until 500 cc. of the leachate is obtained. The leachate is concentrated to about 100 cc., and Ca is precipitated in it as Ca oxalate. The precipitate is filtered and washed until the washings run free from chloride. The precipitate is rejected. The filtrate and washings are evaporated to dryness with 1 cc. of 1:1 H₂SO₄. The residue is ignited to remove NH₄ salts and then dissolved in dilute HCl. The solution is made up to 250 cc. and Mg, Na, K are estimated in 75-cc. aliquots. These are calculated as meqs./100 g. of the soil. The soil on the filter which has been leached with NH₄OAc is saturated with 10 cc. of 0.5N NH₄Cl solution. It is then washed with 40% EtOH adjusted to 7.05 with NH₄OH until the washings run free of chloride. The washed ammonium soil is distilled with MgO, and the NH₃ liberated is estimated in the usual method by absorption in standard H₂SO₄. From the volume of standard H₂SO₄ used the base-exchange capacity of the soil can be calculated. In calcareous soils it may be assumed that the soil is completely base saturated and that no exchangeable H is present. So if the sum of exchangeable Mg, Na, K is subtracted from the base-exchange capacity the amount of exchangeable Ca is obtained.

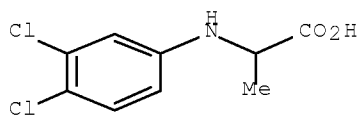
IT 22212-57-3P, Alanine, N-[3,4-dichlorophenyl]-

RL: PREP (Preparation)

(preparation of)

RN 22212-57-3 ZCAPLUS

CN Alanine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)



L68 ANSWER 10 OF 10 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:530132 ZCAPLUS Full-text
 DOCUMENT NUMBER: 75:130132
 ORIGINAL REFERENCE NO.: 75:20560h,20561a
 TITLE: N,N-Disubstituted amino acid herbicides
 INVENTOR(S): Yates, John; Payne, David H.
 PATENT ASSIGNEE(S): Shell Oil Co.
 SOURCE: U.S., 6 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 3598859	A	19710810	US 1967-694116	19671228
GB 1164160	A	19690917	GB 1966-58406	19661230
FR 1575558	A	19690725	FR 1967-1575558	19671228
CH 498087	A	19701031	CH 1967-498087	19671228
DK 123025	B	19720508	DK 1967-6557	19671228
DE 1643527	C3	19791011	DE 1967-S113544	19671228
DE 1643527	B2	19790222		
US 3712805	A	19730123	US 1970-66094	19700821
PRIORITY APPLN. INFO.:			GB 1966-58406	A 19661230
			US 1967-694116	A3 19671228

GI For diagram(s), see printed CA Issue.

AB Numerous N,N-disubstituted amino acid derivs. (I, R = alkyl, aryl or cycloalkyl, R1 = OH, OEt, NHMe, X = halogen, nitro, alkyl, or alkoxy, and n = 1 or 2) were prepared and used as herbicides for controlling undesirable plant growth, especially wild oat. When N-benzoyl-N-(3,4-dichlorophenyl)alanine Et ester (I, X = 3,4-Cl2, R = Ph, R1 = Et), prepared by treating 3,4-dichloroaniline with 2-chloropropionic acid in the presence of Na2CO3, esterifying the product with EtOH, and then treating the product with BzCl, was incorporated into herbicidal compns., it effectively controlled the growth of wild oat.

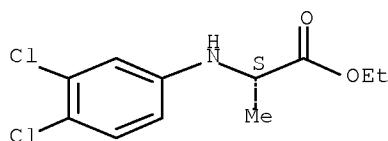
IT 33878-52-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 33878-52-3 ZCAPLUS

CN L-Alanine, N-(3,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



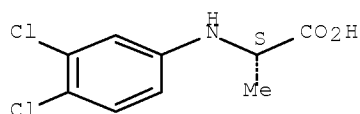
10/598508

ACCESSION NUMBER: 1971:530132 ZCAPLUS Full-text
 DOCUMENT NUMBER: 75:130132
 ORIGINAL REFERENCE NO.: 75:20560h,20561a
 TITLE: N,N-Disubstituted amino acid herbicides
 INVENTOR(S): Yates, John; Payne, David H.
 PATENT ASSIGNEE(S): Shell Oil Co.
 SOURCE: U.S., 6 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3598859	A	19710810	US 1967-694116	19671228
GB 1164160	A	19690917	GB 1966-58406	19661230
FR 1575558	A	19690725	FR 1967-1575558	19671228
CH 498087	A	19701031	CH 1967-498087	19671228
DK 123025	B	19720508	DK 1967-6557	19671228
DE 1643527	C3	19791011	DE 1967-S113544	19671228
DE 1643527	B2	19790222		
US 3712805	A	19730123	US 1970-66094	19700821
PRIORITY APPLN. INFO.:			GB 1966-58406	A 19661230
			US 1967-694116	A3 19671228

GI For diagram(s), see printed CA Issue.
 AB Numerous N,N-disubstituted amino acid derivs. (I, R = alkyl, aryl or cycloalkyl, R1 = OH, OEt, NHMe, X = halogen, nitro, alkyl, or alkoxy, and n = 1 or 2) were prepared and used as herbicides for controlling undesirable plant growth, especially wild oat. When N-benzoyl-N-(3,4-dichlorophenyl)alanine Et ester (I, X = 3,4-Cl2, R = Ph, R1 = Et), prepared by treating 3,4-dichloroaniline with 2-chloropropionic acid in the presence of Na2CO3, esterifying the product with EtOH, and then treating the product with BzCl, was incorporated into herbicidal compns., it effectively controlled the growth of wild oat.
 IT 33878-51-2F
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 33878-51-2 ZCAPLUS
 CN L-Alanine, N-(3,4-dichlorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.



L70 ANSWER 8 OF 8 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1958:29791 ZCAPLUS Full-text
 DOCUMENT NUMBER: 52:29791
 ORIGINAL REFERENCE NO.: 52:5319h-i,5320a-i,5321a-b
 TITLE: Synthesis of ring-substituted N-phenylglycines, their

nitriles, and amides
 AUTHOR(S): Takeda, Akira
 CORPORATE SOURCE: Okayama, Univ., Kurasaki
 SOURCE: Journal of Organic Chemistry (1957), 22, 1096-1100
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 52:29791

AB A series of 14 new 2,4-, 3,4-, and 2,4,5-substituted N-phenylglycines (I), RR'R''C₆H₂NHCH₂CO₂H, was synthesized from the corresponding arylamine (II), RR'R''HC₆H₂NH₂, through the Na N-arylaminoethanesulfonate (III), RR'R''C₆H₂NHCH₂SO₃Na, N-arylglycinonitrile (IV), RR'R''C₆H₂NHCH₂CN, and N-arylglycinamide (V), RR'R''C₆H₂NHCH₂CONH₂. Preliminary biol. testing by the Went pea test (C.A. 29, 22047) indicated that all I and V were active as plant growth substances. NaHSO₃ (375 g.) in 600 ml. H₂O stirred with gradual addition of 243 g. com. 37% HCHO and the mixture refluxed 10 min., filtered, and the filtrate made up to 1 l. with H₂O gave 3M HCHO-NaHSO₃ (VI). Br (32 g.) added slowly with stirring in 10 min. with rise of temperature to 60° to 36.6 g. 3,4-ClMeC₆H₃NHAc in 100 ml. AcOH and the mixture stirred 40 min. at 50-60°, poured slowly into 2 l. cold H₂O containing 6 g. NaHSO₃, and filtered yielded 47 g. 2,4,5-BrMeClC₆H₂NHAc, m. 153-4°(alc.), saponified with 20% NaOH to give pure II (R = Br, R' = Me, R'' = Cl) (VIa), m. 91-2° (alc.), deaminated to colorless material, b₄₀ 116-19°, oxidized with excess KMnO₄ in alkaline solution to authentic 2,5-ClBrC₆H₃CO₂H, m. 157-8°. All tabulated compds. were prepared by essentially the procedures illustrated in the following detailed preps. VI (100 ml.) and 28.2 g. II (R = H, R' = Me, R'' = Cl) (VIb) refluxed 25 min. and the clear solution steam-distilled, the cooled distilland filtered, and the residue washed twice with 50 ml. alc. gave 47 g. methanesulfonate (VIc). KCN (7.2 g.) in 20 ml. H₂O added to 25.7 g. VIc in 50 ml. hot H₂O and the mixture refluxed 40 min., the cooled mixture filtered, and the product dried several days at room temperature in vacuo and 1 day at 40° gave IV (R = H, R' = Me, R'' = Cl) (VId), m. 62-3° (alc.). VIb (28.2 g.) in 40 ml. alc. stirred vigorously with 13.5 g. KCN in 35 ml. H₂O and 1 g. 30% aqueous KOH and the mixture refluxed 6 hrs. with stirring and addition of 16.2 g. 37% HCO, the mixture steam-distilled to recover 5.1 g. unreacted VIb and the distilland concentrated to 50 ml. on a steam bath, the concentrate treated with active C and filtered, the cooled filtrate adjusted to pH 4.0 with 1:1 HCl-H₂O and the mixture stored several hrs., filtered with suction, and the residue dried 12 hrs. at 60° gave 19.5 g. I (R = H, R' = Me, R'' = Cl) (VIe), m. 125-6° (decomposition) (dilute alc.) (method A). VId (3.6 g.) refluxed 3 hrs. with 60 ml. 5% aqueous NaOH and the cooled hydrolyzate filtered gave 0.3 g. V (R = H, R' = Me, R'' = Cl) (VIf), m. 152-3°. Treatment of the filtrate by concentration and acidification as above yielded 86% VIe (method B). VId (3.6 g.) and 60 ml. 1% aqueous NaOH stirred vigorously several min. at 94-5° until NH₃ was evolved, heating continued 20 min. and the cooled solution filtered, the impure product repeatedly extracted with 20 ml. hot H₂O and the white needles (2.6 g.) recrystd. from dilute alc. yielded VIf. Acidification of the filtrate gave 20% VIe. Cautious addition of a small excess of NH₄Et₂ to I in alc. and recrystn. from 1:1 EtOH-NH₄Et₂, gave analytically pure diethylamine salts (VII) of I. The properties and yields of I, VII, III, IV and V with their responses to the Went pea test (C.A. 29, 22047) were tabulated [I (R, R', R''), pH at which I were precipitated, m.p. (decomposition), % yields by methods A and B with % recovered II in parentheses, m.p. VII, and threshold min. concns. in mg./l. exhibiting activity in pea test given]: Cl, Cl, H, 5.2-5.4, 151-2°, 72(33), 87(-), 88-90°, 1.90; H, Cl, Cl, 5.2-5.4, 128-9°, 83(25), 82(7), 137-8°, 0.23; H, Cl, Me, 4.2-4.4, 125-6°, 60(18), 86(8), 120-1°, 6.02; H, Me, Cl, 4.2-4.4, 115-17°, -(-), 69(6), 134-4.5°, 3-22; Br, Me, H, 6.5-5.8, 169-70°, 54(66), 78(8), 123-4°,

6.30; Me, Br, H, 4.8-5, 142-5°, -(-), 82(6), 109-11°, 10.70; Cl, Me, H, 4.2-4.6, 161-4°, 31(71), 91(-), 110-11°, 20.20; Me, Cl, H, 4.2-4.4, 143-4°, 57(52), 83(5), 109-10°, 7.30; Cl, Br, H, 5.6-5.8, 156-7°, -(-), 90(3), 107-8°, 4.20; Br, Cl, H, 5.6-5.8, 163-4°, -(-), 87(6), 118-18.5°, 5.02; Cl, Cl, Cl, 4-4.2, 185-6°, 89(54), 62(8), 174-5°, 0.35; Cl, Me, Cl, 4.6-4.8, 173-5°, -(-), 83(4), 141-3°, 14.50; Br, Me, Cl, 6.2-6.4, 195-6°, -(-), 85(4), 170-4°, 14.70; H, Me, NO₂, 3.8-4.2, 147-9°, -(-), 82(6), 149-50°, 4.52; H, Cl, NO₂, 3.8-4, 174.5-5°, -(-), 67(17), 128-9°, 0.79. [III (R, R', R''), reaction time in min., and % yield on consumed I with % recovered I in parentheses given]: Cl, Cl, H, 120, 87(23); H, Cl, Cl, 25, 94(0); H, Me, Cl, 25, 91(1); H, Cl, Me, 25, 90(0); Br, Me, H, 60, 88(7); Me, Br, H, 40, 99.5(0); Cl, Me, H, 120, 84(8); Me, Cl, H, 120, 90(16); Cl, Br, H, 120, 86(44); Br, Cl, H, 120, 69(51); Cl, Cl, Cl, 180, 38(84); Cl, Me, Cl, 180, 42(71); Br, Me, Cl, 180, 82(83); H, Me, NO₂, 20, 84(0); H, Cl, NO₂, 20, 87(0). [IV (R, R', R''), m.p., and % yield given]: Cl, Cl, H, 76-8°, 87; H, Cl, Cl, 101-2°, 95; H, Me, Cl, 62-3°, 91; H, Cl, Me, 86-7°, 83; Br, Me, H, 62-3°, 89; Me, Br, H, 104.5-5.5°, 89; Cl, Me, H, 47-8°, 83; Me, Cl, H, 101-1.5°, 86; Cl, Br, H, 81-2°, 90; Br, Cl, H, 104-5°, 94; Cl, Cl, Cl, 122-3°, 91; Cl, Me, Cl, 110-12°, 91; Br, Me, Cl, 121-2°, 74; H, Me, NO₂, 101-2°, 99; H, Cl, NO₂, 90.5-1.5°, 92. [V (R, R', R''), m.p. (decomposition), % yield and % IV converted to I in parentheses, and pea test activity given]: Cl, Cl, H, 141-2°, 27(5), 1.36; H, Cl, Cl, 139-9.5°, 49(37), 0.25; H, Me, Cl, 152-3°, 66(2), 4.55; H, Cl, Me, 122-3°, 38(36), 6.40; Br, Me, H, 149.5-50.5°, 38(45), 10.80; Me, Br, H, 156-7°, 40(39), 20.20; Cl, Me, H, 134-5°, 18(55), 42.25; Me, Cl, H, 152.5-4°, 37(48), 3.86; Cl, Br, H, 150-1°, 46(45), 4.43; Br, Cl, H, 144-6°, 44(51), 2.85; Cl, Cl, Cl, 152-3°, 47(31), 0.27; Cl, Me, Cl, 156-7°, 55(24), 10.10; Br, Me, Cl, 167-8°, 44(40), -; H, Me, NO₂, 143.5-4°, 48(36), 5.18; H, Cl, NO₂, 141-2°, 48(33), 1.05. Neither of the Cl atoms in the most active I (R = H, R' = Cl, R'' = Cl) (VIIa) can be replaced by an Me group without loss of biol. activity whereas the o-Cl atom in I (R = Cl, R' = Cl, R'' = H) (VIIb) can be replaced. I (R = R' = R'' = Cl) is as active as VIIa and the replacement of the p-Cl atom in VIIb is accompanied by considerable decrease in biol. activity.

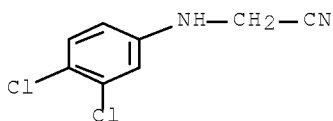
IT 28363-22-6P, Glycinonitrile, N-[3,4-dichlorophenyl]-

RL: PREP (Preparation)

(preparation of)

RN 28363-22-6 ZCAPLUS

CN Acetonitrile, [(3,4-dichlorophenyl)amino]- (9CI) (CA INDEX NAME)



L71 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:425391 ZCAPLUS Full-text

DOCUMENT NUMBER: 81:25391

ORIGINAL REFERENCE NO.: 81:4093a, 4096a

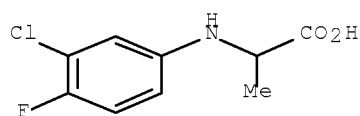
TITLE: Herbicidal alkyl 2-[benzoyl(3-chloro-4-fluorophenyl)amino]propionates

INVENTOR(S): Haddock, Ernest; Sampson, Alan J.

10/598508

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.
 SOURCE: Ger. Offen., 13 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2349970	A1	19740418	DE 1973-2349970	19731004
DE 2349970	C2	19820916		
CA 1006003	A1	19770301	CA 1973-180776	19730911
BE 805652	A1	19740404	BE 1973-136333	19731004
NL 7313634	A	19740409	NL 1973-13634	19731004
FR 2202079	A1	19740503	FR 1973-35490	19731004
ZA 7307784	A	19740828	ZA 1973-7784	19731004
DD 108444	A5	19740920	DD 1973-173869	19731004
JP 49132232	A	19741218	JP 1973-111047	19731004
JP 56024641	B	19810608		
IT 998709	B	19760220	IT 1973-29737	19731004
CS 166653	B2	19760329	CS 1973-6840	19731004
GB 1437711	A	19760603	GB 1973-6464	19731004
ES 419329	A1	19760716	ES 1973-419329	19731004
CH 583507	A5	19770114	CH 1973-14188	19731004
DK 135712	B	19770613	DK 1973-5404	19731004
NO 138882	C	19781129	NO 1973-3866	19731004
NO 138882	B	19780821		
SU 664527	A3	19790525	SU 1973-1962504	19731004
SE 409704	B	19790903	SE 1973-13560	19731004
PRIORITY APPLN. INFO.:			GB 1972-46223	A 19721006
			GB 1973-6464	A 19730209
AB	3,4-ClFC6H3NBzCHMeCO2R (R = Me or CHMe2), used for the control of Avena fatua in cereal cultures, especially wheat and barley, were prepared by benzylation of 3,4-Cl-FC6H3NHCHMeCO2R (I) with BzCl in PhMe at reflux. I were prepared from 3,4-ClFC6H3NH2 and ClCHMe2CO2H via 3,4-ClFC6- H3NHCHMeCO2H, followed by esterification.			
IT	52756-23-7P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
RN	52756-23-7 ZCAPLUS			
CN	Alanine, N-(3-chloro-4-fluorophenyl)- (CA INDEX NAME)			

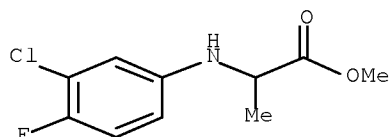


L72 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1974:425391 ZCAPLUS Full-text
 DOCUMENT NUMBER: 81:25391
 ORIGINAL REFERENCE NO.: 81:4093a,4096a

10/598508

TITLE: Herbicidal alkyl 2-[benzoyl(3-chloro-4-fluorophenyl)amino]propionates
 INVENTOR(S): Haddock, Ernest; Sampson, Alan J.
 PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.
 SOURCE: Ger. Offen., 13 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2349970	A1	19740418	DE 1973-2349970	19731004
DE 2349970	C2	19820916		
CA 1006003	A1	19770301	CA 1973-180776	19730911
BE 805652	A1	19740404	BE 1973-136333	19731004
NL 7313634	A	19740409	NL 1973-13634	19731004
FR 2202079	A1	19740503	FR 1973-35490	19731004
ZA 7307784	A	19740828	ZA 1973-7784	19731004
DD 108444	A5	19740920	DD 1973-173869	19731004
JP 49132232	A	19741218	JP 1973-111047	19731004
JP 56024641	B	19810608		
IT 998709	B	19760220	IT 1973-29737	19731004
CS 166653	B2	19760329	CS 1973-6840	19731004
GB 1437711	A	19760603	GB 1973-6464	19731004
ES 419329	A1	19760716	ES 1973-419329	19731004
CH 583507	A5	19770114	CH 1973-14188	19731004
DK 135712	B	19770613	DK 1973-5404	19731004
NO 138882	C	19781129	NO 1973-3866	19731004
NO 138882	B	19780821		
SU 664527	A3	19790525	SU 1973-1962504	19731004
SE 409704	B	19790903	SE 1973-13560	19731004
PRIORITY APPLN. INFO.:			GB 1972-46223	A 19721006
			GB 1973-6464	A 19730209
AB	3,4-ClFC6H3NBzCHMeCO2R (R = Me or CHMe2), used for the control of Avena fatua in cereal cultures, especially wheat and barley, were prepared by benzoylation of 3,4-Cl-FC6H3NHCHMeCO2R (I) with BzCl in PhMe at reflux. I were prepared from 3,4-ClFC6H3NH2 and ClCHMe2CO2H via 3,4-ClFC6- H3NHCHMeCO2H, followed by esterification.			
IT	52756-26-0P			
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
RN	52756-26-0 ZCAPLUS			
CN	Alanine, N-(3-chloro-4-fluorophenyl)-, methyl ester (CA INDEX NAME)			



10/598508

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(FILE 'HOME' ENTERED AT 10:34:02 ON 10 JUN 2008)

FILE 'REGISTRY' ENTERED AT 10:34:14 ON 10 JUN 2008
ACT ZAREKL3L9L12/A

L1 STR
L2 SCR 1867
L3 STR
L4 STR
L5 SCR 616
L6 SCR 1944
L7 SCR 1992
L8 SCR 2004 OR 2021 OR 1993
L9 SCR 868
L10 SCR 877
L11 2640 SEA SSS FUL (L1 AND L3 AND L4) AND (L2 AND L5 AND L6 AND L7
AND L8 AND L9 AND L10)

D L1
D L3
D L4

FILE 'ZCAPLUS' ENTERED AT 10:39:05 ON 10 JUN 2008
L12 812 SEA ABB=ON PLU=ON L11

FILE 'REGISTRY' ENTERED AT 10:39:43 ON 10 JUN 2008

FILE 'STNGUIDE' ENTERED AT 10:48:27 ON 10 JUN 2008

FILE 'REGISTRY' ENTERED AT 10:59:22 ON 10 JUN 2008
L13 STRUCTURE UPLOADED
L14 50 SEA SUB=L11 SSS SAM L13
L15 STRUCTURE UPLOADED
L16 50 SEA SUB=L11 SSS SAM L15
L17 STRUCTURE UPLOADED
L18 50 SEA SUB=L11 SSS SAM L17
L19 STRUCTURE UPLOADED
L20 50 SEA SUB=L11 SSS SAM L19
L21 STRUCTURE UPLOADED
L22 24 SEA SUB=L11 SSS SAM L21
L23 654 SEA SUB=L11 SSS FUL L21
SAVE TEMP L23 ZAR508STR21B/A

FILE 'ZCAPLUS' ENTERED AT 11:28:24 ON 10 JUN 2008
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L25 ANALYZE PLU=ON L24 1- RN HIT : 479 TERMS
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FILE 'REGISTRY' ENTERED AT 13:06:09 ON 10 JUN 2008
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L27 1 SEA ABB=ON PLU=ON 65051-17-4
L28 1 SEA ABB=ON PLU=ON 22212-58-4
L29 1 SEA ABB=ON PLU=ON 22212-57-3
L30 1 SEA ABB=ON PLU=ON 33878-52-3
L31 1 SEA ABB=ON PLU=ON 33878-51-2
L32 1 SEA ABB=ON PLU=ON 28363-22-6

10/598508

L33 1 SEA ABB=ON PLU=ON 52756-23-7
L34 1 SEA ABB=ON PLU=ON 52756-26-0
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FILE 'ZCAPLUS' ENTERED AT 13:09:38 ON 10 JUN 2008

L35 110 SEA ABB=ON PLU=ON L24 AND P/DT
L36 71 SEA ABB=ON PLU=ON L24 NOT L35
L37 86 SEA ABB=ON PLU=ON L35 AND PD<20040303
L38 90 SEA ABB=ON PLU=ON L35 AND PRD<20040303
L39 88 SEA ABB=ON PLU=ON L35 AND AD<20040303
L40 67 SEA ABB=ON PLU=ON L36 AND PY<2005
L*** DEL 0 S L36 AND PRY<2005
L41 159 SEA ABB=ON PLU=ON (L37 OR L38 OR L39 OR L40)

FILE 'REGISTRY' ENTERED AT 13:11:18 ON 10 JUN 2008

L42 645 SEA ABB=ON PLU=ON L23 NOT (L26 OR L27 OR L28 OR L29 OR L30
OR L31 OR L32 OR L33 OR L34)

FILE 'ZCAPLUS' ENTERED AT 13:11:30 ON 10 JUN 2008

L43 144 SEA ABB=ON PLU=ON L42
L44 123 SEA ABB=ON PLU=ON L41 AND L43

FILE 'REGISTRY' ENTERED AT 13:14:52 ON 10 JUN 2008

L45 623 SEA ABB=ON PLU=ON L23 AND X/ELS
L46 358 SEA ABB=ON PLU=ON L23 AND F/ELS
L47 266 SEA ABB=ON PLU=ON L23 AND (?CYANO?/CNS OR ?NITRIL?/CNS)
L48 429 SEA ABB=ON PLU=ON (L46 OR L47)
L49 65 SEA ABB=ON PLU=ON L23 AND C3/ESS
L50 437 SEA ABB=ON PLU=ON (L48 OR L49)

FILE 'ZCAPLUS' ENTERED AT 13:17:52 ON 10 JUN 2008

L51 95 SEA ABB=ON PLU=ON L50

FILE 'REGISTRY' ENTERED AT 13:18:04 ON 10 JUN 2008

FILE 'REGISTRY' ENTERED AT 13:32:04 ON 10 JUN 2008

L52 STRUCTURE UPLOADED
L53 24 SEA SUB=L23 SSS SAM L52
D SCA
L54 613 SEA SUB=L23 SSS FUL L52

FILE 'ZCAPLUS' ENTERED AT 13:37:22 ON 10 JUN 2008

L55 170 SEA ABB=ON PLU=ON L54
D COST FULL
L56 153 SEA ABB=ON PLU=ON L41 AND L55

FILE 'REGISTRY' ENTERED AT 13:38:32 ON 10 JUN 2008

L57 604 SEA ABB=ON PLU=ON L54 NOT (L26 OR L27 OR L28 OR L29 OR L30
OR L31 OR L32 OR L33 OR L34)

FILE 'ZCAPLUS' ENTERED AT 13:38:49 ON 10 JUN 2008

L58 131 SEA ABB=ON PLU=ON L57

10/598508

L59 ANALYZE PLU=ON L58 1- RN HIT : 444 TERMS
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FILE 'REGISTRY' ENTERED AT 13:40:30 ON 10 JUN 2008

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L61 10 SEA ABB=ON PLU=ON L60
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 D RN 2
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FILE 'ZCAPLUS' ENTERED AT 13:41:27 ON 10 JUN 2008

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L65 16 SEA ABB=ON PLU=ON L27
L66 15 SEA ABB=ON PLU=ON L28
L67 14 SEA ABB=ON PLU=ON L29
L68 10 SEA ABB=ON PLU=ON L30
L69 9 SEA ABB=ON PLU=ON L31
L70 8 SEA ABB=ON PLU=ON L32
L71 7 SEA ABB=ON PLU=ON L33
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L73 19 SEA ABB=ON PLU=ON L41 AND L64
L74 14 SEA ABB=ON PLU=ON L41 AND L65
L75 15 SEA ABB=ON PLU=ON L41 AND L66
L76 14 SEA ABB=ON PLU=ON L41 AND L67
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L78 9 SEA ABB=ON PLU=ON L41 AND L69
L79 8 SEA ABB=ON PLU=ON L41 AND L70
L80 7 SEA ABB=ON PLU=ON L41 AND L71
L81 6 SEA ABB=ON PLU=ON L41 AND L72

FILE 'REGISTRY' ENTERED AT 13:45:21 ON 10 JUN 2008

FILE 'ZCAPLUS' ENTERED AT 13:45:28 ON 10 JUN 2008

D STAT QUE L58
D IBIB ABS HITSTR L58 TOT
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D IBIB ABS HITSTR L72 7

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 8 JUN 2008 HIGHEST RN 1026666-11-4
DICTIONARY FILE UPDATES: 8 JUN 2008 HIGHEST RN 1026666-11-4

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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<http://www.cas.org/support/stngen/stndoc/properties.html>

FILE ZCAPLUS

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FILE COVERS 1907 - 10 Jun 2008 VOL 148 ISS 24

FILE LAST UPDATED: 9 Jun 2008 (20080609/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

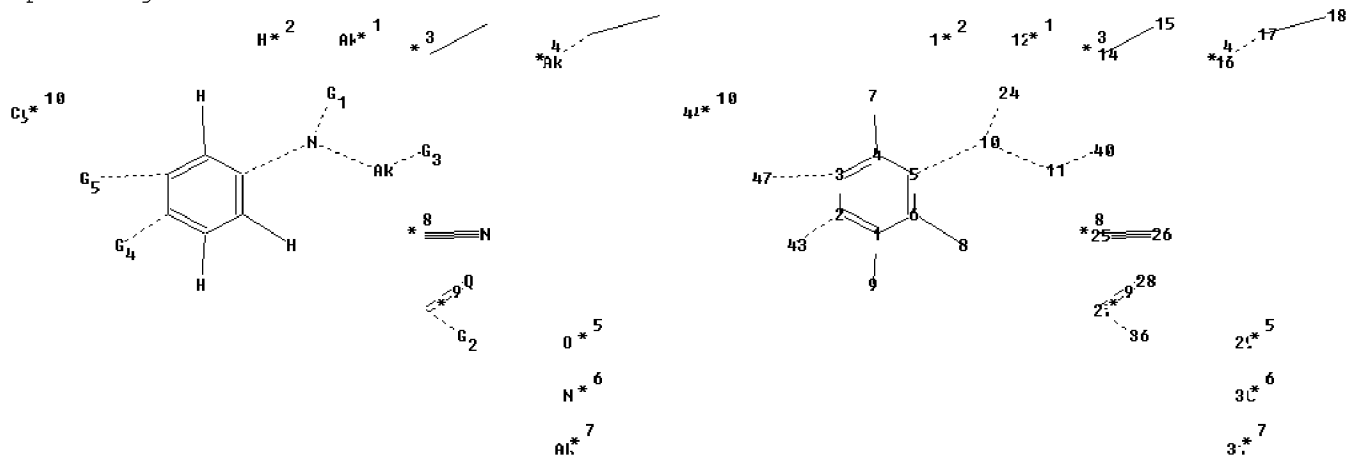
FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jun 6, 2008 (20080606/UP).

=>

Uploading L1b.str



chain nodes :

7 8 9 10 11 12 13 16 24 25 26 27 28 29 31 36 40 43 44 47

ring nodes :

1 2 3 4 5 6 14 15 17 18

ring/chain nodes :

30

chain bonds :

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1-9 2-43 3-47 4-7 5-10 6-8 10-11 10-24 11-40 16-17 25-26 27-28 27-36

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 17-18

exact/norm bonds :

2-43 3-47 5-10 10-11 10-24 11-40 16-17 25-26 27-28 27-36

exact bonds :

1-9 4-7 6-8 14-15 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7]

G3:[*8],[*9]

G4:CN,NO2,X

G5:CN,NO2,O,X,Ak,[*10]

Connectivity :

11:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom

24:CLASS 25:CLASS

26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 36:CLASS 40:CLASS

43:CLASS 44:Atom

47:CLASS

Generic attributes :

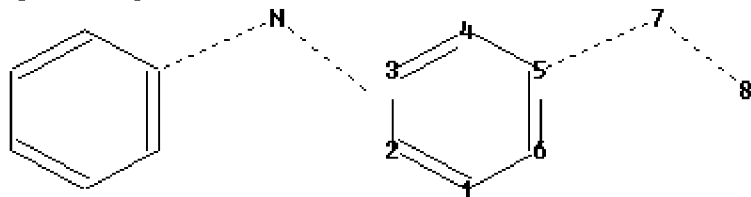
11:

Saturation : Saturated

44:

Saturation : Unsaturated

Uploading L3b.str



chain nodes :

7 8

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

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exact/norm bonds :

5-7 7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

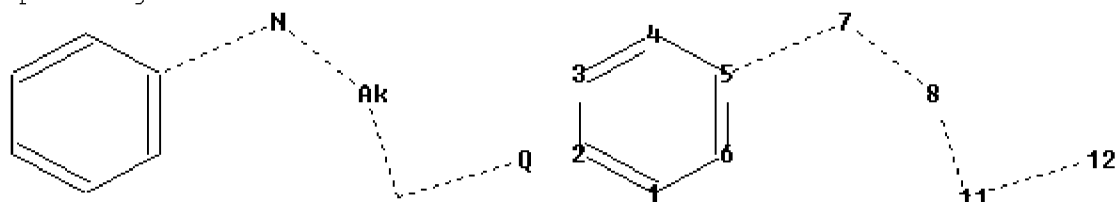
Connectivity :

1:2 E exact RC ring/chain 4:2 E exact RC ring/chain 6:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS

Uploading L4b.str



chain nodes :

7 8 11 12

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 7-8 8-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

5-7 7-8 8-11 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Connectivity :

1:2 E exact RC ring/chain 4:2 E exact RC ring/chain 6:2 E exact RC ring/chain

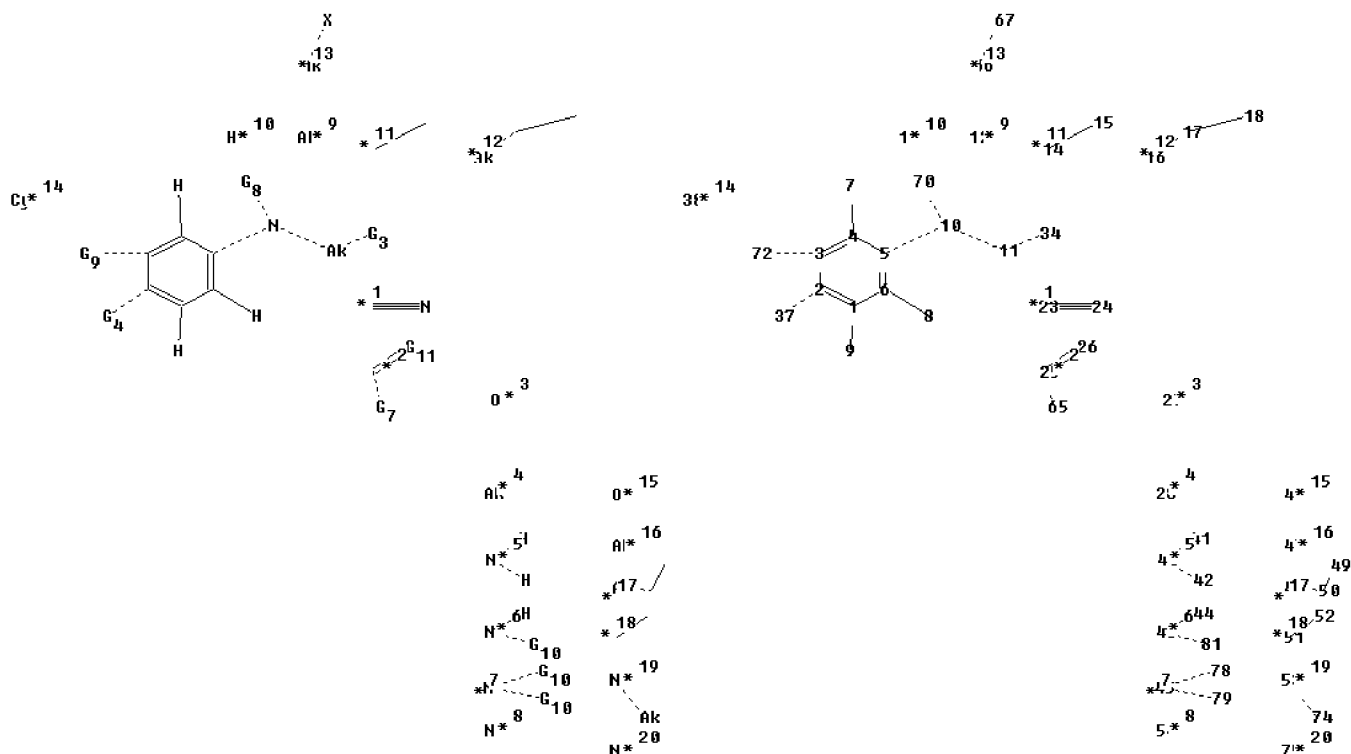
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 11:CLASS

12:CLASS

Uploading L21b.str

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chain nodes :

7 8 9 10 11 12 13 16 23 24 25 26 27 28 34 37 38 40 41 42 43
44 45 46 47 48 53 65 66 67 70 72 74 75 78 79 81

ring nodes :

1 2 3 4 5 6 14 15 17 18 49 50 51 52 54

chain bonds :

1-9 2-37 3-72 4-7 5-10 6-8 10-11 10-70 11-34 16-17 23-24 25-26 25-65
40-41 40-42 43-44 43-81 45-78 45-79 48-50 53-74 66-67

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 17-18 49-50 51-52

exact/norm bonds :

2-37 3-72 5-10 10-11 10-70 11-34 16-17 23-24 25-26 25-65 40-41 40-42
43-44 43-81 45-78 45-79 48-50 53-74 66-67

exact bonds :

1-9 4-7 6-8 14-15 17-18 49-50 51-52

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G3:[*1],[*2]

G4:CN,NO2,X

G7:[*3],[*4],[*5],[*6],[*7],[*8]

G8:[*9],[*10],[*11],[*12],[*13]

G9:CN,NO2,X,O,[*9],[*14],[*13]

G10:[*15],[*16],[*17],[*18],[*19],[*20]

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G11:O,S, [*19], [*20]

Connectivity :

12:1 E exact RC ring/chain 47:1 E exact RC ring/chain 74:1 E exact RC ring/chain

75:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom

23:CLASS 24:CLASS

25:CLASS 26:CLASS 27:CLASS 28:CLASS 34:CLASS 37:CLASS 38:Atom 40:CLASS

41:CLASS 42:CLASS

43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:Atom 50:Atom

51:Atom 52:Atom 53:CLASS

54:Atom 65:CLASS 66:CLASS 67:CLASS 70:CLASS 72:CLASS 74:CLASS 75:CLASS

78:CLASS 79:CLASS

81:CLASS

Generic attributes :

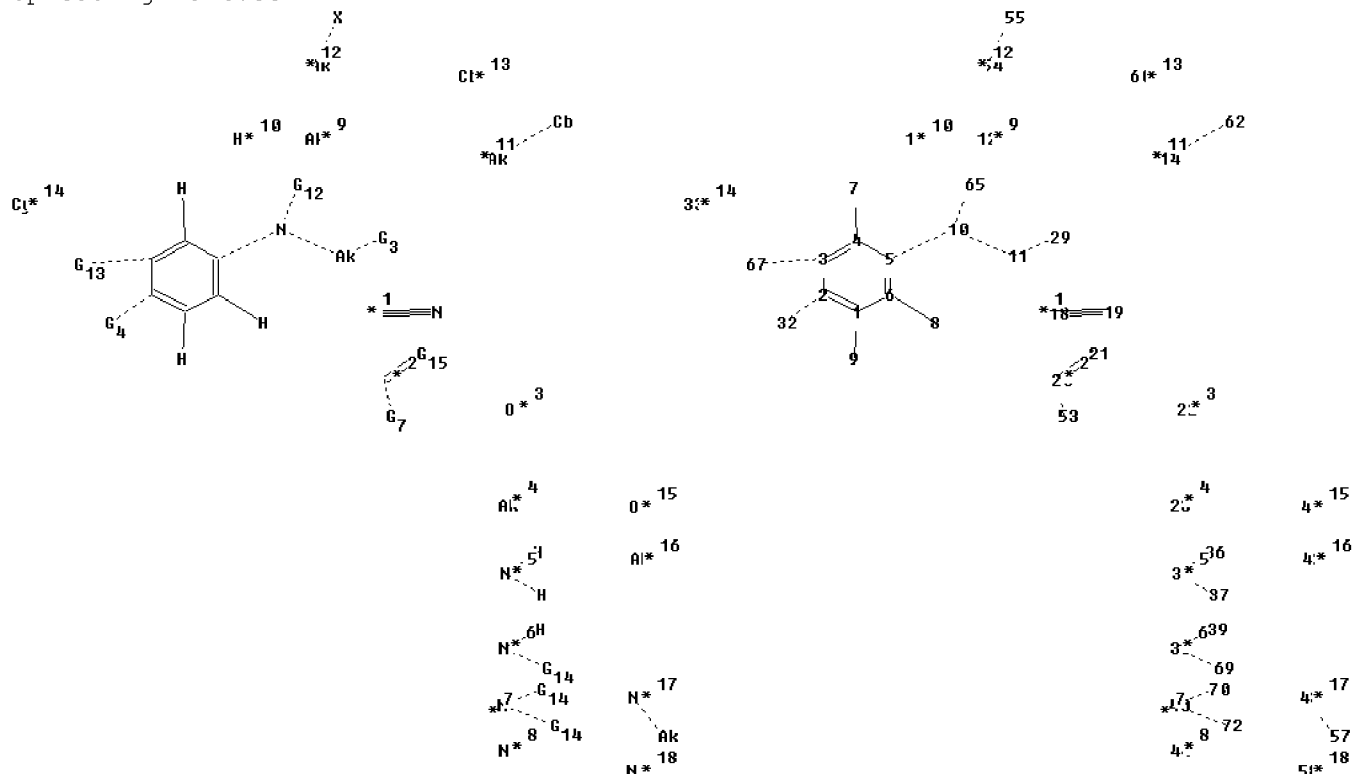
11:

Saturation : Saturated

38:

Saturation : Unsaturated

Uploading L52b.str



chain nodes :

7 8 9 10 11 12 13 14 18 19 20 21 22 23 29 32 33 35 36 37 38
39 40 41 42 43 53 54 55 57 58 60 62 65 67 69 70 72

ring nodes :

1 2 3 4 5 6 44

chain bonds :

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1-9 2-32 3-67 4-7 5-10 6-8 10-11 10-65 11-29 14-62 18-19 20-21 20-53
35-36 35-37 38-39 38-69 40-70 40-72 43-57 54-55

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

2-32 3-67 5-10 10-11 10-65 11-29 14-62 18-19 20-21 20-53 35-36 35-37
38-39 38-69 40-70 40-72 43-57 54-55

exact bonds :

1-9 4-7 6-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G3:[*1],[*2]

G4:CN,NO2,X

G7:[*3],[*4],[*5],[*6],[*7],[*8]

G12:[*9],[*10],[*11],[*12],[*13]

G13:O,CN,NO2,X,[*9],[*14],[*12]

G14:[*11],[*15],[*16],[*17],[*18],[*13]

G15:O,S,[*17],[*18]

Connectivity :

12:1 E exact RC ring/chain 14:2 E exact RC ring/chain 23:1 E exact RC ring/chain
33:1 E exact RC ring/chain 42:1 E exact RC ring/chain 57:1 E exact RC ring/chain
60:1 E exact

RC ring/chain 62:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS
29:CLASS 32:CLASS 33:Atom 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS
40:CLASS 41:CLASS
42:CLASS 43:CLASS 44:Atom 53:CLASS 54:CLASS 55:CLASS 57:CLASS 58:CLASS
60:CLASS 62:Atom
65:CLASS 67:CLASS 69:CLASS 70:CLASS 72:CLASS

Generic attributes :

11:

Saturation : Saturated

33:

Saturation : Unsaturated